

Estimating spectral density functions for Sturm-Liouville problems with two singular endpoints

CHARLES FULTON

Department of Mathematical Sciences
Florida Institute of Technology
Melbourne, Florida 32901-6975

DAVID PEARSON

Department of Mathematics
University of Hull
Cottingham Road
Hull, HU6 7RX England

STEVEN PRUESS

1133 N Desert Deer Pass
Green Valley, Arizona 85614-5530

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Abstract

In this paper we consider the Sturm-Liouville equation $-y'' + qy = \lambda y$ on the half line $(0, \infty)$ under the assumptions that $x = 0$ is a regular singular point and nonoscillatory for all real λ , and that either (i) q is L_1 near $x = \infty$, or (ii) q' is L_1 near ∞ with $q(x) \rightarrow 0$ as $x \rightarrow \infty$, so that there is absolutely continuous spectrum in $(0, \infty)$. Characterizations of the spectral density function for this doubly singular problem, similar to those obtained in [12] and [13] (when the left endpoint is regular) are established; corresponding approximants from the two algorithms in [12] and [13] are then utilized, along with Frobenius recurrence relations and piecewise trigonometric - hyperbolic splines, to generate numerical approximations to the spectral density function associated with the doubly singular problem on $(0, \infty)$. In the case of the radial part of the separated hydrogen atom problem, the new algorithms are capable of achieving near machine precision accuracy over the range of λ from 0.1 to 10000, accuracies which could not be achieved using the SLEDGE software package.

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1 Introduction

In this paper we consider the Sturm-Liouville equation,

$$-y'' + q(x)y = \lambda y, \quad (1.1)$$

on $(0, \infty)$, with two singular endpoints on the half line $(0, \infty)$ under the same assumptions as in [10, 14] under which $x = 0$ is a regular singular point of type **LC/N** or **LP/N** (limit circle or limit point and nonoscillatory at $x = 0$ for all real λ) and $x = \infty$ is of type **LP/O-N** with cutoff $\Lambda = 0$ (limit point and nonoscillatory at $x = \infty$ for $\lambda \in (-\infty, 0)$ and oscillatory for $\lambda \in (0, \infty)$); see [15, p. 114] for these definitions of endpoint classifications developed in connection with the **SLEDGE** software package. Under these assumptions, the spectrum is simple and the eigenfunction expansion associated with equation (1.1) has the general form

$$\begin{aligned} f(x) &= \int_{-\infty}^{\infty} T(\lambda) \cdot \phi(x, \lambda) d\rho(\lambda) \\ &= \sum_{\lambda_n \leq 0} \left[\frac{\int_0^{\infty} f(t) \phi(t, \lambda_n) dt}{\|\phi(t, \lambda_n)\|^2} \right] \phi(x, \lambda_n) + \int_0^{\infty} T(\lambda) \cdot \phi(x, \lambda) d\rho(\lambda) \end{aligned} \quad (1.2)$$

where

$$T(\lambda) := \lim_{b \rightarrow \infty} \int_0^b f(x) \phi(x, \lambda) dx, \quad (1.3)$$

and the solution $\phi(\cdot, \lambda)$ is a suitably normalized Frobenius solution near the regular singular point $x = 0$.

If we make, in addition to the above assumptions, the more stringent assumptions posed in [12] (see **Assumption 3** below), then there is absolutely continuous (a.c.) spectrum in $(0, \infty)$, and the spectral function $\rho(\lambda)$ in (1.2) is absolutely continuous on all closed intervals in $(0, \infty)$.

The purpose of this paper is **(i)** to extend the analysis in [12, 13] under suitable assumptions on $q(x)$ to show that the spectral density function associated with (1.2) over the a.c. range $(0, \infty)$, that is,

$$f(\lambda) = \rho'(\lambda), \quad \rho(\lambda) = \int_0^{\lambda} f(\mu) d\mu \quad (1.4)$$

can be represented for all $\lambda \in (0, \infty)$ as (see **Theorem 3** below)

$$f(\lambda) = \frac{1}{\pi[P(x, \lambda)\phi(x, \lambda)^2 + Q(x, \lambda)\phi(x, \lambda)\phi'(x, \lambda) + R(x, \lambda)\phi'(x, \lambda)^2]}. \quad (1.5)$$

where $(P(\cdot, \lambda), Q(\cdot, \lambda), R(\cdot, \lambda))^T$ is the unique solution of the initial value problem at $x = \infty$:

$$\frac{dU}{dx} = \frac{d}{dx} \begin{bmatrix} P \\ Q \\ R \end{bmatrix} = \begin{bmatrix} 0 & \lambda - q & 0 \\ -2 & 0 & 2(\lambda - q) \\ 0 & -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} P \\ Q \\ R \end{bmatrix}. \quad (1.6)$$

$$\lim_{x \rightarrow \infty} \begin{pmatrix} P(x, \lambda) \\ Q(x, \lambda) \\ R(x, \lambda) \end{pmatrix} = \begin{pmatrix} \sqrt{\lambda} \\ 0 \\ \frac{1}{\sqrt{\lambda}} \end{pmatrix}, \quad \lambda \in (0, \infty), \quad (1.7)$$

and **(ii)** to extend the numerical algorithms from [12, 13] for the computation of the spectral density

function $f(\lambda)$. We illustrate the new numerical algorithms on several examples, including the radial part of the separated hydrogen atom. For the first objective (i) we make use of the fact that $f(\lambda)$ is characterized as the boundary value of a suitable Titchmarsh-Weyl m -function by the Titchmarsh-Kodaira formula, which was recently established for such doubly singular problems in [16, 14] (see **Theorem 2** below). For the second objective (ii) we make use of exact Frobenius power series to estimate the solution $\phi(x, \lambda)$ and its derivative near $x = 0$, and then apply initial conditions at a suitable point $x_0(\lambda) > 0$ using values of $\phi(x_0(\lambda), \lambda)$ and $\phi'(x_0(\lambda), \lambda)$ which can generally be computed to machine precision, so that numerical algorithms from [12, 13] with the left endpoint regular can be adapted to approximate the right hand side of (1.5); this is done by shooting with piecewise trigonometric / hyperbolic splines to compute the solution ϕ of (1.1) and the solution $(P, Q, R)^T$ of (1.6) at a suitable ‘matching’ point $x \in (x_0(\lambda), \infty)$.

The organization of topics needed in this paper to accomplish the above two objectives is as follows: In section 2 we give the main assumptions near $x = 0$ from [10, 14], and the general forms of two linearly independent Frobenius power series solutions in all the cases we consider in this paper. In section 3 we list (without proof) the elementary results which relate and interconnect solutions of the Sturm-Liouville equation (1.1) with solutions of Appell’s first order system (1.6); none of these elementary results require any special assumptions on the potential q . In section 4 we add the main assumptions from [12] under which the initial value problem (1.6)-(1.7) has a unique solution in $(0, \infty)$, and reformulate in terms of solutions of Appell’s system (1.6) results obtained by D.B. Pearson and his student Al-Naggar in [1, 2]. This yields the spectral density function characterization (1.5) in the relatively simple case of a regular left endpoint. In contrast to [1, 2] we do not focus the analysis on the third order ordinary differential equation (see (4.13) below) which is satisfied by the third component, $R(x, \lambda)$, of (1.6), but make use instead of many of the elegant formulas from section 2. In section 5 we generalize the methods of [1, 2] to the doubly singular problem on $(0, \infty)$, when the m -function is defined relative to the suitably normalized Frobenius fundamental system as in [10, 14]. This yields **Theorem 3** below (a new result) in which the new Titchmarsh-Kodaira formula (see **Theorem 2** below) for the (single) spectral density function associated with the doubly singular problem gets converted to the form (1.5). In section 6 we list four test examples of equations on $(0, \infty)$ from [10, 14] for which explicit closed form formulas for the spectral density function were obtained. In section 7 we describe how the two different types of numerical algorithms from [12] and [13] (for cases involving a regular left endpoint) can be adapted, using appropriate heuristics, to yield new algorithms for computing the spectral density function when both endpoints are singular, which is done by utilizing the characterization (1.5) in an appropriate way. In section 8 we give numerical output showing that the new algorithms for doubly singular problems can achieve very high accuracy on the four test examples in section 6; we also give numerical output demonstrating convergence of our numerical approximations for a potential on $(0, \infty)$ from quantum chemistry where the potential has an infinite series representation satisfying all our assumptions. In section 9 we make use of our new code, AutoB, for the spectral density computation in order to generate, by quadratures, approximations to the spectral functions for the four examples in section 6, and give comparisons on timing and accuracy with the corresponding **SLEDGE** runs. Our main conclusion is that the new algorithms for doubly singular problems are very much superior to the older algorithms for doubly singular problems which were implemented in the **SLEDGE** software package.

Remark. In our previous papers [12, 13] the system (1.6) was referred to as the “PQR equations” (our notation); however, the analysis leading to them (particularly the motivating property (3.14)) was discovered by M. Appell [3] in 1880. Accordingly, we will henceforth refer to this first order system as the Appell equations.

2 Suitably Normalized Frobenius Solutions

In this section we repeat the basic definitions and some of the elementary properties of the suitably normalized Frobenius solutions which were introduced in Fulton [10] and Fulton and Langer [14]. It will be noted that, in most of the common cases (Bessel equations, Confluent Hypergeometric equations, Whittaker equations) rather standard normalizations of well known special functions have to be abandoned in order to achieve the desired analytic properties of the Frobenius solutions (particularly, entire

behaviour in λ) needed for the fundamental definition of a single Titchmarsh-Weyl m -function, the corresponding scalar spectral function, and for determination of eigenfunction expansions of the problems considered in this paper (all of which have simple spectrum).

We consider in this paper the Sturm-Liouville equation (1.1) on the half line $(0, \infty)$ under the following assumptions (see [10, 14]):

Assumption 1: Near $x = 0$:

Case I: For all $x \in (0, \infty)$,

$$q(x) = \frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n, \quad q_n \text{ real for all } n, \quad (2.1)$$

where the series is convergent in $(0, \infty)$, and where

$$-\frac{1}{4} \leq q_0 < \infty. \quad \text{and } q_0, q_1 \text{ not both zero.} \quad (2.2)$$

or

Case II: There exists $a > 0$ such that $q(x)$ is given by (2.1) for $x \in (0, a]$ where the series is convergent in $(0, a]$ and where (2.2) holds, and in the interval $[a, \infty)$ we have $q \in L_{loc}^1[a, \infty)$,

and

Assumption 2: Near $x = \infty$:

$$\lim_{x \rightarrow \infty} q(x) = 0, \quad (2.3)$$

The assumptions near $x = 0$ ensure that the indicial roots near the regular singular point $x = 0$ are both real; it follows that the endpoint $x = 0$ is either **LC/N** or **LP/N**, and the assumption near $x = \infty$ ensure that the endpoint $x = \infty$ is **LP/O-N** with cutoff $\Lambda = 0$ in the terminology of [15]. Under the above assumptions it was proved in [10, Theorems 4.2, 4.3, 5.3, 5.4] and [14, Theorem 4.5] that the eigenfunction expansion associated with (1.1) (in both the **LP** and **LC** cases at $x = 0$ assumes the form (1.2), with a suitably normalized Frobenius solution $\phi(\cdot, \lambda)$.

We now give the formulas for all cases of Frobenius solutions which can occur at $x = 0$ under the assumptions (2.1)-(2.2); these are the solutions which were utilized in [10, 14]. The indicial equation for the R.S.P. $x = 0$ for the Sturm-Liouville equation (1.1) with potential (2.1),

$$-y''(x) + \left(\frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n \right) y(x) = \lambda y(x), \quad x \in (0, \infty). \quad (2.4)$$

is

$$r^2 - r - q_0 = r^2 - r - \left(\nu^2 - \frac{1}{4} \right) = \left(r - \left(\frac{1}{2} + \nu \right) \right) \cdot \left(r - \left(\frac{1}{2} - \nu \right) \right) \quad (2.5)$$

where we have set

$$q_0 = \nu^2 - \frac{1}{4}, \nu \geq 0$$

for convenience. This gives rise to the following cases of Frobenius solutions:

Case I: $-\frac{1}{4} < q_0 < \infty$, $q_0 = \nu^2 - \frac{1}{4} \neq \frac{M^2-1}{4}$, $M = 1, 2, \dots$ (This is Case IA in [10]). In this case,

$$y_1(x, \lambda) = x^{\frac{1}{2}+\nu} \left(1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n \right), \quad (2.6)$$

$$y_2(x, \lambda) = x^{\frac{1}{2}-\nu} \left(1 + \sum_{n=1}^{\infty} b_n(\lambda)x^n \right), \quad (2.7)$$

where $a_n(\lambda), b_n(\lambda)$ are polynomials in λ of degree $\lfloor \frac{n}{2} \rfloor$, and

$$W_x(y_1(\cdot; \lambda), y_2(\cdot; \lambda)) = -2\nu. \quad (2.8)$$

Case II A: $q_0 = \frac{M^2-1}{4}$, M odd: $M = 2\ell + 1$, $\ell = 0, 1, \dots$, that is, $q_0 = \ell(\ell + 1)$.

In [10] this is Case IC for M odd and it includes Case II (for $\ell = 0$). In this case,

$$y_1(x, \lambda) = x^{\ell+1} \left(1 + \sum_{n=1}^{\infty} a_n(\lambda) x^n \right), \quad (2.9)$$

$$y_2(x, \lambda) = K_\ell(\lambda) y_1(x; \lambda) \ln x + x^{-\ell} \left(1 + \sum_{n=1}^{\infty} d_n(\lambda) x^n \right), \quad (2.10)$$

where $a_n(\lambda), d_n(\lambda)$ are polynomials in λ of degree $\lfloor \frac{n}{2} \rfloor$, $K_\ell(\lambda)$ is a polynomial of degree ℓ , and

$$W_x(y_1(\cdot, \lambda), y_2(\cdot, \lambda)) = -(2\ell + 1). \quad (2.11)$$

Case II B: $q_0 = \frac{M^2-1}{4}$, M even: $M = 2N$, $N = 0, 1, \dots$, that is, $q_0 = N^2 - \frac{1}{4}$.

In [10] this is Case IC for M even and it includes Case IB (for $N = 0$). In this case,

$$y_1(x, \lambda) = x^{\frac{1}{2}+N} \left(1 + \sum_{n=1}^{\infty} a_n(\lambda) x^n \right), \quad (2.12)$$

$$y_2(x, \lambda) = y_1(x, \lambda) \ln x + \sum_{n=1}^{\infty} d_n(\lambda) x^{\frac{1}{2}+n}, \quad \text{if } N = 0$$

$$y_2(x, \lambda) = K_N(\lambda) y_1(x; \lambda) \ln x + x^{\frac{1}{2}-N} \left(1 + \sum_{n=1}^{\infty} d_n(\lambda) x^n \right), \quad \text{if } N \geq 1 \quad (2.13)$$

where $a_n(\lambda), d_n(\lambda)$ are polynomials in λ of degree $\lfloor \frac{n}{2} \rfloor$, $K_N(\lambda)$ is a polynomial of degree N , and

$$W_x(y_1(\cdot, \lambda), y_2(\cdot, \lambda)) = \begin{cases} -2N & \text{if } N \geq 1, \\ 1 & \text{if } N = 0. \end{cases} \quad (2.14)$$

In each of the above cases the first Frobenius solution $y_1(\cdot, \lambda)$ is the principal solution at $x = 0$ for all $\lambda \in (-\infty, \infty)$. The Frobenius solutions as normalized above satisfy the following properties (see [10, Theorem 2.1]):

- (i) $y_1(x, \cdot), y_2(x, \cdot)$ and their derivatives are entire functions for each $x \in (0, \infty)$ and satisfy for all $\lambda \in \mathbb{C}$, $x \in (0, \infty)$ the relations

$$y_i(x, \bar{\lambda}) = \overline{y_i(x, \lambda)}, \quad y'_i(x, \bar{\lambda}) = \overline{y'_i(x, \lambda)}, \quad i = 1, 2.$$

- (ii) $y_1(\cdot, \lambda) \in L_2(0, x_0)$ for $0 < x_0 < \infty$ and for all $\lambda \in \mathbb{C}$.

- (iii) $W_x(y_1(\cdot, \lambda), y_2(\cdot, \lambda)) = C \neq 0$ where $C \in \mathbb{R}$, independent of λ .

It follows that a fundamental system of solutions near $x = 0$ which is entire in λ and satisfies property (i), together with the normalization

$$W_x(\phi(\cdot, \lambda), \theta(\cdot, \lambda)) = 1 \quad \text{for all } \lambda \in \mathbb{C}, \quad (2.15)$$

can be selected by taking

$$\phi(x, \lambda) := y_1(x, \lambda), \quad \theta(x, \lambda) := y_2(x, \lambda)/C, \quad (2.16)$$

where C is the real constant in (2.8), (2.11), or (2.14). In the **LP** cases at $x = 0$ only $\phi(\cdot, \lambda)$ satisfies the property (ii) of square integrability near $x = 0$, so in all **LP** cases it is the first Frobenius solution which is used to write the eigenfunction expansion in the form (1.2).

The **LC** cases at $x = 0$ are Case I with $q_0 \in (-\frac{1}{4}, 0) \cup (0, \frac{3}{4})$, Case IIA with $q_0 = 0(\ell = 0)$, and Case IIB with $q_0 = \frac{1}{4}(N = 0)$. In this paper we limit our consideration of **LC** boundary conditions at $x = 0$ to the Friedrichs **LC** boundary condition (see (5.2) below); in this case it is the first Frobenius solution ϕ (the principal solution) which is selected and used in the eigenfunction expansion (1.2).

3 Preliminaries

In this section we collect together some useful results which relate solutions of the Sturm-Liouville equation (1.1) to solutions of the companion first order system (1.6). The proofs of these results (though sometimes tedious) require only straightforward algebraic manipulation making use of these two equations, and no special assumptions on the potential $q(x)$; so we omit the proofs.

1. If y is any solution of the SL-equation, then $((y')^2, -2yy, y^2)^T$ is a solution of the first order system (1.6).

2. If we let a fundamental system of the Sturm-Liouville equation (2.4) be defined by the initial conditions at any $x_0 > 0$

$$\begin{bmatrix} u(x_0, \lambda) & v(x_0, \lambda) \\ u'(x_0, \lambda) & v'(x_0, \lambda) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad (3.1)$$

then a corresponding fundamental system of solutions of equation (1.6) is

$$U = [U_1, U_2, U_3] = \begin{bmatrix} (u')^2 & u'v' & (v')^2 \\ -2uu' & -[u'v + uv'] & -2vv' \\ u^2 & uv & v^2 \end{bmatrix}. \quad (3.2)$$

3. If $\{\phi(x, \lambda), \theta(x, \lambda)\}$ are the Frobenius solutions defined in Section 2 (in all the cases) and normalized by (2.16) so as to ensure that $W_x(\phi(\cdot, \lambda), \theta(\cdot, \lambda)) = 1$, then a corresponding fundamental system of solutions of equation (1.6) is

$$U = [U_1, U_2, U_3] = \begin{bmatrix} (\theta')^2 & \theta'\phi' & (\phi')^2 \\ -2\theta\theta' & -[\theta'\phi + \theta\phi'] & -2\phi\phi' \\ \theta^2 & \theta\phi & \phi^2 \end{bmatrix} \quad (3.3)$$

4. An indefinite inner product on the solution space of equation (1.6) may be defined by

$$\langle U_1, U_2 \rangle := 2(P_1R_2 + P_2R_1) - Q_1Q_2 = \text{const}, \text{ independent of } x \in [0, \infty) \quad (3.4)$$

where $U_k = (P_k, Q_k, R_k), k = 1, 2$.

5. For any solution $U = (P, Q, R)^T$ of equation (1.6),

$$\frac{d}{dx} \langle U, U \rangle = \frac{d}{dx} [4PR - Q^2] = 0,$$

i.e.

$$4PR - Q^2 = \text{const}, \text{ independent of } x \in [0, \infty) \quad (3.5)$$

6. If U_1 and U_2 are any two solutions of equation (1.6) represented in the form,

$$U_j = \begin{bmatrix} P_j \\ Q_j \\ R_j \end{bmatrix} = a_j \begin{bmatrix} (\theta')^2 \\ -2\theta\theta' \\ \theta^2 \end{bmatrix} + b_j \begin{bmatrix} \theta'\phi' \\ -[\theta'\phi + \theta\phi'] \\ \theta\phi \end{bmatrix} + c_j \begin{bmatrix} (\phi')^2 \\ -2\phi\phi' \\ \phi^2 \end{bmatrix} \quad (3.6)$$

in terms of the Frobenius solutions $\{\phi(\cdot, \lambda), \theta(\cdot, \lambda)\}$ of section 2, then we have

$$\langle U_1, U_2 \rangle := 2(P_1R_2 + P_2R_1) - Q_1Q_2 = 2(a_1c_2 + c_1a_2) - b_1b_2 \quad (3.7)$$

In particular,

$$\langle U_1, U_1 \rangle := 4P_1R_1 - Q_1^2 = 4a_1c_1 - b_1^2. \quad (3.8)$$

7. Similarly, if these same solutions, U_1 and U_2 , of equation (1.6) are represented in the form,

$$U_j = \begin{bmatrix} \tilde{P}_j \\ \tilde{Q}_j \\ \tilde{R}_j \end{bmatrix} = \tilde{a}_j \begin{bmatrix} (u')^2 \\ -2uu' \\ u^2 \end{bmatrix} + \tilde{b}_j \begin{bmatrix} u'v' \\ -[uv' + u'v] \\ uv \end{bmatrix} + \tilde{c}_j \begin{bmatrix} (v')^2 \\ -2vv' \\ v^2 \end{bmatrix} \quad (3.9)$$

in terms of the solutions defined in (3.1)-(3.2) we have

$$\langle U_1, U_2 \rangle := 2(\tilde{P}_1 \tilde{R}_2 + \tilde{P}_2 \tilde{R}_1) - \tilde{Q}_1 \tilde{Q}_2 = 2(\tilde{a}_1 \tilde{c}_2 + \tilde{c}_1 \tilde{a}_2) - \tilde{b}_1 \tilde{b}_2. \quad (3.10)$$

In particular,

$$\langle U_1, U_1 \rangle := 4\tilde{P}_1 \tilde{R}_1 - \tilde{Q}_1^2 = 4\tilde{a}_1 \tilde{c}_1 - \tilde{b}_1^2. \quad (3.11)$$

It follows from (3.7), (3.10) and (3.8), (3.11) that we must also have

$$2(a_1 c_2 + c_1 a_2) - b_1 b_2 = 2(\tilde{a}_1 \tilde{c}_2 + \tilde{c}_1 \tilde{a}_2) - \tilde{b}_1 \tilde{b}_2, \quad \text{and } 4a_1 c_1 - b_1^2 = 4\tilde{a}_1 \tilde{c}_1 - \tilde{b}_1^2. \quad (3.12)$$

8. If y is any solution of the SL equation (1.1) and $U=(P,Q,R)^T$ is any solution of the companion system (1.6) then

$$\frac{d}{dx}[Py^2 + Qyy' + R(y')^2] = 0, \quad (3.13)$$

i.e.,

$$P(x, \lambda)y^2(x, \lambda) + Q(x, \lambda)y(x, \lambda)y'(x, \lambda) + R(x, \lambda)(y'(x, \lambda))^2 = \text{constant, independent of } x. \quad (3.14)$$

4 A Spectral Density Function Characterization of Al-Naggar and Pearson

In this section we consider the Sturm-Liouville problem

$$-y''(x) + \left(\frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n \right) y(x) = \lambda y(x), \quad x \in [A, \infty), \quad A > 0, \quad (4.1)$$

$$y(A) = 0. \quad (4.2)$$

We shall assume that **Assumption 1, Case I**, holds, so that the above potential q is continuous in $(0, \infty)$ and also has a continuous derivative. In addition we make the following assumption:

Assumption 3: Near $x = \infty$:

For $x_0 > 0$ we have either

$$q \in L_1(x_0, \infty) \quad (4.3)$$

or

$$q' \in L_1(x_0, \infty), \quad q \in AC_{loc}[x_0, \infty), \quad \text{and } \lim_{x \rightarrow \infty} q(x) = 0. \quad (4.4)$$

Under the assumption (4.3) or the assumption (4.4) it was established in Fulton, Pearson and Pruess [12, Thm1 and Cor 2] that the initial value problem (1.6)-(1.7) has a unique solution for all $\lambda \in (0, \infty)$. Henceforth we denote this unique solution by

$$U_1(x, \lambda) = \begin{bmatrix} P_1(x, \lambda) \\ Q_1(x, \lambda) \\ R_1(x, \lambda) \end{bmatrix}, \quad (4.5)$$

that is, U_1 is the unique solution (under **Assumption 3**) for which

$$\lim_{x \rightarrow \infty} U_1(x, \lambda) = \begin{pmatrix} P_1(\infty, \lambda) \\ Q_1(\infty, \lambda) \\ R_1(\infty, \lambda) \end{pmatrix} = \begin{pmatrix} \sqrt{\lambda} \\ 0 \\ \frac{1}{\sqrt{\lambda}} \end{pmatrix}, \quad \text{for } \lambda \in (0, \infty).$$

The assumptions (4.3) and (4.4) were used in [12, 13] to obtain spectral density function characterizations of the type (1.5) when the left endpoint is regular. Al-Naggar and Pearson [1, 2] also obtained a spectral density function characterization of this type when the left endpoint is regular, using a different

approach. Their approach was based on the determination of intervals of a.c. spectrum by locating those intervals of the real λ -axis where subordinate solutions do not exist. The purpose of this section is to present their analysis as it applies to the problem (4.1)-(4.2) and under the additional **Assumption 3** on the half line $[A, \infty)$, $A > 0$, and show that it also guarantees a.c. spectrum for $\lambda \in (0, \infty)$ and yields a spectral density function formula of the type (1.5) (see (4.30) below and [12, Cor 4]); this route to the spectral density function characterization represents an alternative to the analysis in [12, 13]. As we shall see, the approach of Al-Naggat and Pearson has a major advantage in that it extends nicely to obtain a corresponding spectral density function characterization of the type (1.5) for the doubly singular equation (4.1) on $(0, \infty)$. This will be done in the next section.

In [1, 2] the analysis is focused on the third order ordinary differential equation (see (4.13) below) satisfied by the third component of a solution of Appell's first order system; here, we modify the approach slightly so as to focus attention on the system (1.6), so that we can properly exploit the results from [12] on uniqueness of the above solution U_1 satisfying the initial condition (1.7).

Letting $\{u(\cdot, \lambda), v(\cdot, \lambda)\}$ be the fundamental system of solutions of (4.1) defined by the initial conditions (3.1) at $x_0 = A$, the Titchmarsh-Weyl m-function associated with the problem (4.1)-(4.2) is defined by

$$\Psi_A(\cdot, \lambda) := u(\cdot, \lambda) + m_A(\lambda)v(\cdot, \lambda) \in L_2(A, \infty), \quad \text{for all } \operatorname{Im}(\lambda) \neq 0. \quad (4.6)$$

Then, as is well known, this m-function is a Nevanlinna function and therefore admits the representation

$$m_A(z) = \alpha + \beta z + \int_{-\infty}^{\infty} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) d\rho_A(t), \quad \alpha \in (-\infty, \infty), \quad \beta \geq 0, \quad (4.7)$$

where the inversion integral for ρ_A in terms of m is the Titchmarsh-Kodaira formula

$$\rho_A(\lambda) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_0^\lambda \operatorname{Im}[m_A(t + i\varepsilon)] dt. \quad (4.8)$$

Since the **Assumption 3** ensures a.c. spectrum for $\lambda \in (0, \infty)$ we may differentiate (4.8) to obtain the spectral density function as

$$f_A(\lambda) := \rho'_A(\lambda) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \operatorname{Im}[m_A(\lambda + i\varepsilon)] \quad (4.9)$$

We now proceed to transform (4.9) into the form (1.5); after some analysis this yields (4.30) in Theorem 1 below. In the sequel it will be helpful to make use of the fundamental system of solutions of Appell's system (1.6) given in (3.2) in terms of the solutions $\{u(\cdot, \lambda), v(\cdot, \lambda)\}$ of equation (4.1) fixed by the initial conditions (3.1) with $x_0 = A$

LEMMA 1. Assume the potential q satisfies **Assumption 3**.

(i) For all $\lambda \in (0, \infty)$ let U_1 be the unique solution defined at $x = \infty$ in (4.5). Then using the indefinite inner product on the solution space of (1.6) defined in (3.7) we have

$$\langle U_1, U_1 \rangle = 4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = 4. \quad (4.10)$$

(ii) If the solution U_1 is represented in the form (3.9), say

$$U_1(x, \lambda) = \begin{bmatrix} P_1(x, \lambda) \\ Q_1(x, \lambda) \\ R_1(x, \lambda) \end{bmatrix} = \tilde{a} \begin{bmatrix} (u')^2 \\ -2uu' \\ u^2 \end{bmatrix} + \tilde{b} \begin{bmatrix} u'v' \\ -[uv' + u'v] \\ uv \end{bmatrix} + \tilde{c} \begin{bmatrix} (v')^2 \\ -2vv' \\ v^2 \end{bmatrix} \quad (4.11)$$

then

$$4\tilde{a}\tilde{b} - (\tilde{c})^2 = 4. \quad (4.12)$$

PROOF.(i) To get the constant 4 observe from (3.5) and the initial condition (1.7) that

$$4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = \lim_{x \rightarrow \infty} 4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = 4\sqrt{\lambda} \cdot \left(\frac{1}{\sqrt{\lambda}} \right) = 4.$$

(ii) The conversion of the indefinite inner product in terms of the coefficients $\{\tilde{a}, \tilde{b}, \tilde{c}\}$ is the property (3.7) and (3.8); this is readily proved by substitution of the components of U_1 into the inner product formula and use of the wronskian relation $W_x(u(\cdot, \lambda), v(\cdot, \lambda)) = 1$. ■

It can be shown that the third component, $R(x, \lambda)$, of a solution of Appell's system (1.6) satisfies the third order equation of [2, p. 6584, Equa. 5],

$$\frac{d^3 R}{dx^3} + 4(\lambda - q(x)) \frac{dR}{dx} - 2q'(x)R = 0. \quad (4.13)$$

Remark In Appell's paper this third order equation is [3, p. 213, Equa (5)].

Also, a general solution of (4.13) can be obtained from a suitably normalized solution $R_1(x, \lambda)$ as in [2, p. 6587, Lemma 2]. Here we generalize this technique to obtain from the given solution U_1 , two other linearly independent solutions. This is the content of the following lemma.

LEMMA 2. Let $U_1 = (P_1, Q_1, R_1)^T$ be the unique solution of (1.6) defined at $x = \infty$ by the initial condition (1.7). Then we can write the general solution of (1.6) in the form

$$U = \begin{bmatrix} P \\ Q \\ R \end{bmatrix} = \beta_1 U_1 + \beta_2 U_2 + \beta_3 U_3, \quad (4.14)$$

where

$$U_2(x, \lambda) = \begin{bmatrix} P_1 \cos 2\gamma + (Q_1/R_1) \sin 2\gamma - (2/R_1) \cos 2\gamma \\ Q_1 \cos 2\gamma + 2 \sin 2\gamma \\ R_1 \cos 2\gamma \end{bmatrix}, \quad (4.15)$$

$$U_3(x, \lambda) = \begin{bmatrix} P_1 \sin 2\gamma - (Q_1/R_1) \cos 2\gamma - (2/R_1) \sin 2\gamma \\ Q_1 \sin 2\gamma - 2 \cos 2\gamma \\ R_1 \sin 2\gamma \end{bmatrix}, \quad (4.16)$$

and

$$\gamma(x) = \int_{x_0}^x 1/R_1(t, \lambda) dt$$

for some $x_0 > 0$.

PROOF. The fact that

$$R(x, \lambda) := R_1(x, \lambda)[\beta_1 + \beta_2 \cos 2\gamma + \beta_3 \sin 2\gamma]$$

is a general solution of (4.13) follows as in [2, Lemma 2, p. 6587]. Since (4.13) is satisfied by the third component of any solution of (1.6), we can generate a general solution for (1.6) by computing $Q(x, \lambda) = -dR/dx$ and then $P(x, \lambda) = [-dQ/dx + 2(\lambda - q)R]/2$ and expressing these solutions of (1.6) in terms of P_1, Q_1, R_1 . This gives the result (4.14). Alternatively, a direct substitution of U_2 and U_3 into (1.6) and use of the formulas for P'_1, Q'_1 and R'_1 will verify that U_2 and U_3 are solutions of (1.6). ■

COROLLARY. (i) The general solution (4.14) in Lemma 2 satisfies

$$\langle U, U \rangle = 4PR - Q^2 = 4((\beta_1)^2 - (\beta_2)^2 - (\beta_3)^2). \quad (4.17)$$

Similarly, if

$$\tilde{U} = (\tilde{P}, \tilde{Q}, \tilde{R}) = \tilde{\beta}_1 U_1 + \tilde{\beta}_2 U_2 + \tilde{\beta}_3 U_3,$$

we have for the inner product that

$$\begin{aligned} \langle U, \tilde{U} \rangle &= 2(P\tilde{R} + R\tilde{P}) - Q\tilde{Q} \\ &= 4(\beta_1\tilde{\beta}_1 - \beta_2\tilde{\beta}_2 - \beta_3\tilde{\beta}_3). \end{aligned} \quad (4.18)$$

(ii) The solutions $\{U_1, U_2, U_3\}$ in Lemma 1 are mutually orthogonal with respect to the indefinite inner product defined in (3.4).

PROOF. (i) For (4.17) calculate $4PR - Q^2$ using (4.14) and the normalization (4.10). This simplifies to

$$\begin{aligned} 4(\beta_1 + \beta_2 \cos 2\gamma + \beta_3 \sin 2\gamma)^2 &= 8(\beta_2 \cos 2\gamma + \beta_3 \sin 2\gamma)(\beta_1 + \beta_2 \cos 2\gamma + \beta_3 \sin 2\gamma) \\ &= 4((\beta_2)^2 \sin^2 2\gamma + (\beta_3)^2 \cos^2 2\gamma - 2\beta_2\beta_3 \sin 2\gamma \cos 2\gamma) \\ &= 4((\beta_1)^2 - (\beta_2)^2 - (\beta_3)^2). \end{aligned}$$

the proof of (4.18) is similar.

(ii) Taking $U = U_1$, which satisfies the normalization (4.10), and $\tilde{U} = U_2$ in (4.15) we have from (4.18) that $\langle U_1, U_2 \rangle = 4(1 \cdot 0 - 0 \cdot 1 - 0 \cdot 0) = 0$. Similarly, $\langle U_1, U_3 \rangle$ and $\langle U_2, U_3 \rangle$ are zero. ■

Remark. The third component, R_1 , of (4.11) satisfies the third order equation (4.13) and since $R_1(x, \lambda) \rightarrow 1/\sqrt{\lambda} > 0$, it is in fact the same quadratic form as $Y(x, \lambda)$ which was employed in [2, Lemma3 and Thm2].

The following lemma gives a limit relation involving the solution, U_1 , and the solutions from Lemma 2 which are orthogonal to it.

LEMMA 3. We assume the potential q satisfies **Assumption 3**.

(i) For the solution U_1 of the initial value problem (1.6)-(1.7), let U_2 and U_3 be the linearly independent solutions of Lemma 1 which are generated by using $(P_1, Q_1, R_1)^T$ in (4.15) and (4.16). Then, for any linear combination

$$U = \begin{pmatrix} P \\ Q \\ R \end{pmatrix} = \beta_2 U_2 + \beta_3 U_3$$

we have for all $x_0 > 0$,

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N R(x, \lambda) dx}{\int_{x_0}^N R_1(x, \lambda) dx} = 0. \quad (4.19)$$

(ii) The representation (4.11) for U_1 has $\tilde{a}(\lambda) > 0$ and $\tilde{c}(\lambda) > 0$ for all $\lambda \in (0, \infty)$.

PROOF (i). The solutions U_2 and U_3 in (4.15) and (4.16) have $R_2 = R_1(x, \lambda) \cos(2\gamma(x))$ and $R_3 = R_1(x, \lambda) \sin(2\gamma(x))$, where

$$\gamma(x) = \int_{x_0}^x [1/R_1(t, \lambda)] dt,$$

for all $x > 0$. The fact that $R_1(x) > 0$ for all $x > 0$ follows from (4.20) below. Consequently, it suffices to prove that (4.19) holds for these two choices of R . For R_2 we have

$$\begin{aligned} \int_{x_0}^N R_1 \cos 2\gamma dx &= \int_{x_0}^N 0.5(R_1)^2 \frac{d}{dx} \sin 2\gamma dx \\ &= 0.5(R_1)^2 \sin 2\gamma \Big|_{x_0}^N + \int_{x_0}^N R_1 Q_1 \sin 2\gamma dx. \end{aligned}$$

Since $Q_1(x) \rightarrow 0$ as $x \rightarrow \infty$ we can prove that

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N R_1 Q_1 \sin 2\gamma dx}{\int_{x_0}^N R_1 dx} = 0.$$

Given $\epsilon > 0$, pick x_ϵ sufficiently large that $|Q_1(x)| < \epsilon$ for $x \geq x_\epsilon$. Then we have

$$\left| \int_{x_0}^N R_1 Q_1 \sin 2\gamma dx \right| \leq M \int_{x_0}^{x_\epsilon} R_1 dx + \epsilon \int_{x_\epsilon}^N R_1 dx,$$

where M is a bound on Q_1 in $[x_0, x_\epsilon]$. Now pick N sufficiently large that

$$\frac{M \int_{x_0}^{x_\epsilon} R_1 dx}{\int_{x_0}^N R_1 dx} < \epsilon,$$

which is possible since $\int_{x_0}^{\infty} R_1 dx = \infty$. Then the above quotient is less than 2ϵ . For the boundary term we have

$$\begin{aligned} [R_1(N, \lambda)]^2 &= [R_1(x_0, \lambda)]^2 + \int_{x_0}^N 2R_1 R_1' dx \\ &= [R_1(x_0, \lambda)]^2 - \int_{x_0}^N 2R_1 Q_1 dx, \end{aligned}$$

so

$$\lim_{N \rightarrow \infty} \frac{[R_1(N, \lambda)]^2}{\int_{x_0}^N R_1 dx} = 0,$$

by employing the same argument. The proof for R_3 is similar.

(ii) In the representation (4.11) for U_1 we have

$$R_1(x, \lambda) = \tilde{a}u(x, \lambda)^2 + \tilde{b}u(x, \lambda)v(x, \lambda) + \tilde{c}v(x, \lambda)^2.$$

To see that $\tilde{a} > 0$ and $\tilde{c} > 0$ for all $\lambda \in (0, \infty)$ we first observe from (4.12) that $4\tilde{a}\tilde{c} - (\tilde{b})^2 = 4$ requires \tilde{a} and \tilde{c} to be of the same sign; and this must hold for all $\lambda \in (0, \infty)$ since they are continuous and cannot pass through zero (which would violate (4.12)). Factoring out \tilde{a} we have

$$R_1(x, \lambda) = \tilde{a}[u(x, \lambda)^2 + (\tilde{b}/\tilde{a})u(x, \lambda)v(x, \lambda) + (\tilde{c}/\tilde{a})v(x, \lambda)^2]$$

with the coefficients of u^2 and v^2 positive. Therefore R_1 admits a factorization of the form

$$\begin{aligned} R_1(x, \lambda) &= \tilde{a}[(u(x, \lambda) + \alpha v(x, \lambda))(u(x, \lambda) + \bar{\alpha} v(x, \lambda))] \\ &= \tilde{a}|u(x, \lambda) + \alpha v(x, \lambda)|^2, \end{aligned} \tag{4.20}$$

where $\alpha = \alpha_1 + i\alpha_2$ must satisfy (by (4.12))

$$\alpha_1 = -\tilde{b}/(2\tilde{a}) \text{ and } \alpha_2^2 = (\tilde{c}/\tilde{a}) - [(\tilde{b})^2/(4(\tilde{a})^2)] = 1/(\tilde{a})^2. \tag{4.21}$$

Since \tilde{a} , \tilde{b} , and \tilde{c} are real, we must have either $\alpha_2 = 1/\tilde{a}$ or $\alpha_2 = -1/\tilde{a}$; but either way the factorization remains the same with α and $\bar{\alpha}$ switched. Since $|u - \alpha v|^2 > 0$, it follows from the above factorization that $\tilde{a}(\lambda) > 0$ for all $\lambda \in (0, \infty)$; otherwise, $\lim_{x \rightarrow \infty} R_1(x, \lambda) \leq 0$ contradicting the fact that $R_1(\infty, \lambda) = 1/\sqrt{\lambda} > 0$. Hence, also $\tilde{c}(\lambda) > 0$ for all $\lambda \in (0, \infty)$. ■

Since the definition of α_2 must be $\pm 1/\tilde{a}(\lambda)$ from (4.21) and since this indeterminacy is actually immaterial, we choose to take $\alpha_2 = 1/\tilde{a}(\lambda)$, so that

$$\alpha(\lambda) := -\frac{\tilde{b}}{2\tilde{a}} + i \frac{1}{\tilde{a}}. \tag{4.22}$$

Using the fundamental system $\{u(\cdot, \lambda), v(\cdot, \lambda)\}$ we now define the complex-valued solution of (4.1) for real $\lambda \in (0, \infty)$,

$$\psi_A(x, \lambda) := u(x, \lambda) + \alpha(\lambda)v(x, \lambda). \tag{4.23}$$

The key idea of Al-Naggar and Pearson, which enables identification of a.c. spectrum, is embodied in the following requirement:

Definition. The general Sturm-Liouville equation (1.1) satisfies *Condition A*, for a given real value of λ , if and only if there exists a complex-valued solution $y(x, \lambda)$ of (1.1) for which

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N y(x, \lambda)^2 dx}{\int_{x_0}^N |y(x, \lambda)|^2 dx} = 0 \quad \text{for } x_0 > 0. \tag{4.24}$$

We now prove that equation (4.1) satisfies *Condition A* for all $\lambda \in (0, \infty)$.

LEMMA 4. Assume $q(x)$ in (4.1) satisfies **Assumptions 3**. Then for $x_0 > 0$ and all $\lambda \in (0, \infty)$

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \psi_A(x, \lambda)^2 dx}{\int_{x_0}^N |\psi_A(x, \lambda)|^2 dx} = 0. \quad (4.25)$$

PROOF: Since equation (4.13) is satisfied by all linear combinations of $v(\cdot, \lambda)^2$, $u(\cdot, \lambda)v(\cdot, \lambda)$ and $u(\cdot, \lambda)^2$ (see [2, Lemma 1, p. 6584]), it follows that $\psi_A(\cdot, \lambda)^2$ is a solution of (4.13) and since it is complex-valued, also that $\text{Re}[\psi_A(\cdot, \lambda)^2]$ and $\text{Im}[\psi_A(\cdot, \lambda)^2]$ satisfy (4.13). Accordingly, it follows that there exist solutions $U_2 = (P_2, Q_2, \text{Re}(\psi_A^2))^T$ and $U_3 = (P_3, Q_3, \text{Im}(\psi_A^2))^T$ of the first order system (1.6), since any real solution R of (4.13) can be used to generate a solution of (1.6) having R as its third component; e.g., let $Q' = -R'$ and $P = -Q'/2 - (\lambda - q)R$. From (4.20) and (4.23) we readily deduce the following representations of $R_1(\cdot, \lambda)$, $\text{Re}[\psi_A(\cdot, \lambda)]^2$, and $\text{Im}[\psi_A(\cdot, \lambda)]^2$ of the form (4.11) (or, the third component of (4.11)):

$$\begin{aligned} R_1(x, \lambda) &= \tilde{a}u^2 + 2\tilde{a}\alpha_1 uv + \tilde{a}(\alpha_1^2 + \alpha_2^2)v^2 \\ \text{Re}[\psi_A(x, \lambda)]^2 &= u^2 + 2\alpha_1 uv + (\alpha_1^2 - \alpha_2^2)v^2 \\ \text{Im}[\psi_A(x, \lambda)]^2 &= 2\alpha_2 uv + 2\alpha_1 \alpha_2 v^2. \end{aligned}$$

It now follows from these formulas that the above solutions U_2 and U_3 associated with $\text{Re}[\psi_A(\cdot, \lambda)]^2$ and $\text{Im}[\psi_A(\cdot, \lambda)]^2$ are orthogonal to U_1 in the sense of the inner product defined in (3.7), i.e., we have

$$\langle U_1, U_2 \rangle = 2[\tilde{a}(\alpha_1^2 - \alpha_2^2) + \tilde{a}(\alpha_1^2 + \alpha_2^2)] - 4\tilde{a}\alpha_1^2 = 0,$$

and

$$\langle U_1, U_3 \rangle = 2[\tilde{a}(2\alpha_1 \alpha_2) + 0] - 4\tilde{a}\alpha_1 \alpha_2 = 0.$$

Hence it follows from Lemma 3(i) that for all $x_0 > 0$

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \text{Re}[\psi_A(x, \lambda)]^2 dx}{\int_{x_0}^N R_1(x, \lambda) dx} = 0$$

and

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \text{Im}[\psi_A(x, \lambda)]^2 dx}{\int_{x_0}^N R_1(x, \lambda) dx} = 0,$$

from which (4.25) follows. \blacksquare

Assumming the Sturm-Liouville equation (1.1) has a potential q which is **LP** at $x = \infty$ and regular at a finite left endpoint, Al-Nagggar and Pearson obtain the following results in [1, Lemma1 and Thm2] (where the fundamental system $\{u, v\}$ is defined by initial conditions at the left endpoint so that v satisfies a general regular boundary condition and $W_x(u(\cdot, \lambda), v(\cdot, \lambda)) = 1$):

LEMMA 5 (*Al-Nagggar and Pearson*). Let $I \subset (-\infty, \infty)$ be an interval on which Condition A holds for the general equation (1.1), and let the fundamental system $\{u(\cdot, \lambda), v(\cdot, \lambda)\}$ be defined by the initial conditions (3.1) at $x_0 = A$. Then

(i) There exists a complex valued function $M(\lambda)$ on I which is uniquely defined by the properties:

$$(a) \quad \text{Im}[M(\lambda)] > 0 \quad \text{and} \quad (b) \quad \lim_{N \rightarrow \infty} \frac{\int_{x_0}^N (u(x, \lambda) + M(\lambda)v(x, \lambda))^2 dx}{\int_{x_0}^N |(u(x, \lambda) + M(\lambda)v(x, \lambda))|^2 dx} = 0.$$

(ii) For $\lambda \in I$ the function M in (i) is the boundary value of the Titchmarsh-Weyl m -function defined by (4.6), that is,

$$M(\lambda) = \lim_{\epsilon \downarrow 0} [m_A(\lambda + i\epsilon)].$$

PROOF. Statements (i) and (ii) are, respectively, Lemma 1 and Theorem 2 from [1]. ■

We now apply these results to the problem (4.1)-(4.2).

LEMMA 6. Assume that for the problem (4.1)-(4.2) **Assumption 3** holds. Then with $\alpha(\lambda)$ defined by (4.22) we have for all $\lambda \in (0, \infty)$

$$\alpha(\lambda) = \lim_{\epsilon \downarrow 0} [m_A(\lambda + i\epsilon)]. \quad \blacksquare \quad (4.26)$$

PROOF. By the uniqueness of $M(\lambda)$, and the fact for all $\lambda \in I = (0, \infty)$ $\alpha(\lambda)$ has positive imaginary part (see (4.22) and Lemma 3(ii)) and $\psi_A(x, \lambda)$ satisfies property (b) in Lemma 5(i) (see Lemma 4) it follows from Lemma 5(ii) with $I = (0, \infty)$ that for all $\lambda \in (0, \infty)$ we must have (4.26). ■

We are now ready to prove the representation of $f_A(\lambda)$ in the form (1.5).

Theorem 1 Assume the potential q is given as in (4.1) and that **Assumption 3** holds. Let $\alpha(\lambda)$ be defined as in (4.22) and $\psi_A(\cdot, \lambda)$ as in (4.23). Then the spectral function defined by (4.8) for the problem (4.1)-(4.2) is absolutely continuous for $\lambda \in (0, \infty)$ and the corresponding spectral density function admits the following representations for $\lambda \in (0, \infty)$:

$$f_A(\lambda) := \rho'(\lambda) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \text{Im}[m(\lambda + i\epsilon)] \quad (4.27)$$

$$= \frac{\alpha_2(\lambda)}{\pi} \quad (4.28)$$

$$= \frac{1}{\pi \tilde{a}(\lambda)} \quad (4.29)$$

$$= \frac{1}{\pi [P_1(x, \lambda)(v(x, \lambda))^2 + Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + R_1(x, \lambda)(v'(x, \lambda))^2]} \quad (4.30)$$

PROOF: The statement (4.28), and the absolute continuity of the spectral function ρ , follows from Lemma 6 by taking imaginary parts on each side of equation (4.26). The statement (4.29) follows from the definition of α_2 in (4.22). To obtain (4.30) substitute $U_1 = (P_1, Q_1, R_1)^T$ from the representation (4.11) in terms of $\{u(x, \lambda), v(x, \lambda)\}$ and collect coefficients of $\tilde{a}(\lambda)$, $\tilde{b}(\lambda)$ and $\tilde{c}(\lambda)$ to obtain

$$Pv^2 + Qvv' + R(v')^2 = \tilde{a}(\lambda)[W_x(v, u)]^2 = \tilde{a}(\lambda).$$

■

Remark. Putting $x = 0$ in (4.30) yields $f_A(\lambda) = 1/(\pi R_1(A, \lambda))$ which was a main result of Theorem 2 in [2].

The following well known spectral density function formula, due to Titchmarsh [23], 1946, and Weyl [24], 1910, in the case of the assumption (4.3) (and due to Pearson [19, 11] in the case of assumption (4.4)) also follows readily from **Theorem 1**:

Corollary. Under the assumptions of **Theorem 1** we have for all $\lambda \in (0, \infty)$

$$f_A(\lambda) = \lim_{x \rightarrow \infty} \frac{1}{\pi [\sqrt{\lambda}(v(x, \lambda))^2 + \frac{1}{\sqrt{\lambda}}(v'(x, \lambda))^2]}. \quad (4.31)$$

PROOF: The **Assumption 3** ensures (see [12, Thm 2]) that the solutions v and u defined by the initial conditions (3.1) are bounded for sufficiently large x . Hence, making use of the initial condition (1.7)

which U_1 satisfies, we have

$$\begin{aligned}
& P_1(x, \lambda)(v(x, \lambda))^2 + Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + R_1(x, \lambda)(v'(x, \lambda))^2 \\
&= \lim_{x \rightarrow \infty} [P_1(x, \lambda)(v(x, \lambda))^2 + Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + R_1(x, \lambda)(v'(x, \lambda))^2] \\
&= \lim_{x \rightarrow \infty} Q_1(x, \lambda)v(x, \lambda)v'(x, \lambda) + \lim_{x \rightarrow \infty} [P_1(x, \lambda)(v(x, \lambda))^2 + R_1(x, \lambda)(v'(x, \lambda))^2] \\
&= 0 + \lim_{x \rightarrow \infty} [\sqrt{\lambda}(v(x, \lambda))^2 + \frac{1}{\sqrt{\lambda}}(v'(x, \lambda))^2],
\end{aligned}$$

so it follows that (4.30) gives rise to the characterization (4.31). \blacksquare

Remark. In [12] we made use of the formula (4.31) to establish (4.30). Here, by linking the spectral density function first to the m-function, and following the approach of Al-Naggar and Pearson, we have obtained a direct proof of (4.30), from which the older result (4.31) follows as a consequence.

5 Generalization of a Spectral Density Function Characterization to Doubly Singular problems

In this section we consider the Sturm-Liouville problem

$$\tau y := -y''(x) + \left(\frac{q_0}{x^2} + \frac{q_1}{x} + \sum_{n=0}^{\infty} q_{n+2}x^n \right) y(x) = \lambda y(x), \quad x \in (0, \infty), \quad (5.1)$$

$$W_0((y(\cdot, \lambda), \phi(\cdot, 0))) = \lim_{x \rightarrow 0} W_x((y(\cdot, \lambda), \phi(\cdot, 0))) = 0, \quad \text{if } x = 0 \text{ is } \mathbf{LC}, \quad (5.2)$$

where $\phi(x, 0)$ is the first Frobenius solution for $\lambda = 0$ given in (2.16). Since this is also the principal solution at $x = 0$ in all (**LC** and **LP**) cases, the boundary condition (5.2) is the Friedrichs boundary condition in the **LC** cases at $x = 0$ and selects $\phi(x, \lambda)$ for all $\lambda \in C$; this boundary condition is also automatically satisfied by $\phi(x, \lambda)$ in all the **LP** cases at $x = 0$. In this section we adopt the **Assumption 1** and **2** from Section 2, and the **Assumption 3** from Section 4. Our aim is to extend the spectral density function characterization in **Theorem 1** (under the above 3 assumptions) to obtain the formula (1.5) for the doubly singular problem (5.1)-(5.2). The **Assumption 1** ensures that $x = 0$ is a singular point of type **LP/N** or **LC/N**; the **Assumption 2** ensures that $x = \infty$ is a singular point of type **LP/O-N** with cutoff value $\Lambda = 0$; and the **Assumption 3** ensures that we have a.c. spectrum in $(0, \infty)$. The underlying self-adjoint operator associated with (5.1)-(5.2) has the domain

$$\begin{aligned}
D(A) := \left\{ f \in L_2(0, \infty) \mid f(x) \in AC_{loc}^1(0, \infty), \tau f \in L_2(0, \infty), \right. \\
\left. \lim_{x \rightarrow 0} W_x(f(\cdot), \phi(\cdot, 0)) = 0 \right\}
\end{aligned} \quad (5.3)$$

in the **LC** cases at $x = 0$, and

$$D(A) := \left\{ f \in L_2(0, \infty) \mid f \in AC_{loc}^1(0, \infty), \tau f \in L_2(0, \infty) \right\} \quad (5.4)$$

in the **LP** cases at $x = 0$. The associated eigenfunction expansion theory which obtains the eigenfunction expansion in the form (1.2) for both of the above cases was given in [10] and [14], and explicit formulas for the corresponding Titchmarsh-Weyl m-function and associated scalar spectral function were obtained in [14] for all cases of the special potential

$$q(x) = \frac{q_0}{x^2} + \frac{q_1}{x}, \quad q_0 \text{ and } q_1 \text{ satisfying (2.2).} \quad (5.5)$$

Here the Titchmarsh-Weyl m-function is defined as in [10, 14] by

$$\Psi(\cdot, \lambda) := \theta(\cdot, \lambda) - m(\lambda)\phi(\cdot, \lambda) \in L_2(x_0, \infty), \quad x_0 > 0, \quad \text{for all } \operatorname{Im}(\lambda) \neq 0. \quad (5.6)$$

where $\phi(\cdot, \lambda)$ and $\theta(\cdot, \lambda)$ are the first and second Frobenius solutions normalized as in (2.16). We now repeat some basic information from [14] concerning the Titchmarsh-Weyl m -functions defined by (5.6). In the **LC** cases at $x = 0$ the m -function defined by (5.6) is a Nevanlinna function (that is, a function of class \mathbf{N}_0), and therefore admits an integral representation of the form (4.7), and the inversion integral for ρ in terms of m is a Titchmarsh-Kodaira formula like (4.8). The eigenfunction expansion for the problem (5.1)-(5.2) when $x = 0$ is **LC** has the form (1.2) where $\phi(\cdot, \lambda)$ is the first Frobenius solution in (2.16), and ρ is the spectral function obtained from the above m -function.

In the **LP** cases at $x = 0$, the m -function defined by (5.6) is a generalized Nevanlinna function of class \mathbf{N}_κ for some $\kappa \geq 1$ (see [14, p. 188]) and it follows using the theory of Krein and Langer [18] for these functions (see [14, Thm 3.5 and Lemma 4.1]) that they admit the representation

$$m(z) = (1 + z^2)^n \int_{-\infty}^{\infty} \left(\frac{1}{t - z} - \frac{t}{1 + t^2} \right) d\sigma(t) + \sum_{j=0}^m \alpha_j z^j$$

where $n, m \geq 1$, $\alpha_j \in (-\infty, \infty)$, $\alpha_m \neq 0$ if $m > 0$, and where σ is a measure on \mathbb{R} satisfying

$$\int_{-\infty}^{\infty} \frac{d\sigma(t)}{1 + t^2} < \infty.$$

The spectral function for the associated self-adjoint operator A in (5.4) is then defined in terms of σ as

$$\rho(\lambda) := \int_0^\lambda (1 + s^2)^n d\sigma(s), \quad \lambda \in (-\infty, \infty). \quad (5.7)$$

While the Titchmarsh-Kodaira formula is well known for \mathbf{N}_0 functions, it was only recently established in various cases with two **LP** endpoints and simple spectrum by Gesztesy and Zinchenko [16] and Fulton and Langer [14]. For the case of equation (5.1), where generalized Nevanlinna functions of class \mathbf{N}_κ arise, we quote this result, and also relate it to the classical real-variable definition of Levitan and Levinson (see [14, Thm 4.7 and 4.8]):

Theorem 2 (*Fulton and Langer*). Consider equation (5.1) with $x = 0$ of **LP** type and suppose **Assumptions 1 and 2** hold. If λ, λ_0 are points of ρ -measure zero (not discrete eigenvalues of the associated self-adjoint operator A), then the spectral function defined by (5.7) has the representation

$$\begin{aligned} \rho(\lambda) - \rho(\lambda_0) &= \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda} \operatorname{Im}[m(\mu + i\epsilon)] d\mu \\ &= \lim_{b \rightarrow \infty} \sum_{\lambda_{jb} \in (\lambda_0, \lambda) \cap \sigma(A_b)} \frac{1}{\int_0^b |\phi(x, \lambda_{jb})|^2 dx}. \end{aligned} \quad (5.8)$$

Note: When (5.1) is of **LC** type at $x = 0$ we have $n = 0$ in (5.7) and a standard Nevanlinna representation of $m(\lambda)$, for which the inversion formula is also (5.8).

Here, A_b is the corresponding truncated self-adjoint operator on $(0, b]$ with any regular boundary condition at $x = b$. It follows from [14, Thm 4.5] that for the **LP** cases at $x = 0$ the function defined by (5.7) or (5.8) is the spectral function which arises in the eigenfunction expansion (1.2). For proofs of convergence results and Parseval relation we refer to [10, 14].

Remark. The above theorem justifies the use of the second formula in (5.8) for the computation of the spectral function ρ as was implemented in the software package **SLEDGE** when both endpoints are of **LP** type. For Sturm-Liouville problems satisfying **Assumptions 1,2** of Section 2, **SLEDGE** [15, Equ (1.13)] does in fact normalize the ϕ -solution as in (2.6), (2.9) and (2.12).

If we make the **Assumption 3** in addition to the assumptions 1 and 2 of Section 2, the spectrum is a.c. on $(0, \infty)$. In the case when the left endpoint is regular, it was shown under **Assumption 3** in [12, Thm 1 and Cor 2] that the initial value problem (1.6)-(1.7) at $x = \infty$ has a unique solution for each of the cases (5.3) and (5.4); also, that the spectral density function has the form (1.5) (see [12, Cor 4]

and [13, Thm 1]) for each of these cases. The proof required linking the formula (1.5) to the well known result of Weyl and Titchmarsh (4.31) in the Corollary to Theorem 1. An alternative approach to the proof of (1.5) when the left endpoint is regular was given by Al-Naggar and Pearson [1, 2] as described in Section 4. We now follow this method of analysis to generalize the above Theorem 1 to the case when both endpoints are singular and all three assumptions hold. Since the spectral function is absolutely continuous in $(0, \infty)$, we may differentiate in (5.8) to obtain the spectral density function as

$$f(\lambda) := \rho'(\lambda) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \text{Im}[m(\lambda + i\epsilon)]. \quad (5.9)$$

The eigenfunction expansion associated with the underlying self-adjoint operator A when $x = 0$ is **LP** has the form (1.2) where $\phi(\cdot, \lambda)$ is the first Frobenius solution in (2.16), and ρ is the spectral function defined in (5.7) or (5.8). In both cases (**LC** and **LP** at $x = 0$) the spectral density function is given by (5.9) in terms of the m -function which is defined in (5.6) above relative to the suitably normalized Frobenius solutions.

We proceed now to transform (5.9) to the form (1.5); after some analysis this yields (5.30) in Theorem 3 below. Since many of the necessary lemmas which are required are the same as in Section 4, we list and prove only those lemmas which undergo some change as a result of allowing the left endpoint $x = 0$ to be a singular endpoint satisfying **Assumptions 1,2**. We also adopt the notational convention that Lemma n^* in this section represents the analog of Lemma n in Section 4.

In the sequel it will be helpful to make use of the fundamental system of solutions of Appell's system (1.6) given in (3.3) in terms of the suitably normalized Frobenius solutions $\{\phi(\cdot, \lambda), \theta(\cdot, \lambda)\}$ of equation (5.1) fixed by the definition (2.16).

LEMMA 1*. Assume that for equation (5.1) **Assumption 1, CaseI**, and **Assumption 2,3** hold.

(i) Same as Lemma 1(i); this yields

$$\langle U_1, U_1 \rangle = 4P_1(x, \lambda)R_1(x, \lambda) - (Q_1(x, \lambda))^2 = 4. \quad (5.10)$$

(ii) If the solution U_1 is represented in the form (3.6), say

$$U_1(x, \lambda) = \begin{bmatrix} P_1(x, \lambda) \\ Q_1(x, \lambda) \\ R_1(x, \lambda) \end{bmatrix} = a^* \begin{bmatrix} (\theta')^2 \\ -2\theta\theta' \\ \theta^2 \end{bmatrix} + b^* \begin{bmatrix} \theta'\phi' \\ -[\theta\phi' + \theta'\phi] \\ \theta\phi \end{bmatrix} + c^* \begin{bmatrix} (\phi')^2 \\ -2\phi\phi' \\ \phi^2 \end{bmatrix} \quad (5.11)$$

then

$$4a^*c^* - (b^*)^2 = 4. \quad (5.12)$$

PROOF. (ii) The conversion of the indefinite inner product in terms of the coefficients $\{a^*, b^*, c^*\}$ is the property (3.7) and (3.8); this is readily proved by substitution of the components of U_1 into the inner product formula and use of the wronskian relation $W_x(\phi(\cdot, \lambda), \theta(\cdot, \lambda)) = 1$. ■

LEMMA 3*. Assume that for equation (5.1) **Assumption 1, CaseI**, and **Assumption 2,3** hold.

(i) Same as Lemma 3(i).

(ii) The representation (5.11) for U_1 has $a^*(\lambda) > 0$ and $c^*(\lambda) > 0$ for all $\lambda \in (0, \infty)$.

PROOF: (ii) In the representation (5.11) for U_1 we have

$$R_1(x, \lambda) = a^*\theta(x, \lambda)^2 + b^*\theta(x, \lambda)\phi(x, \lambda) + c^*\phi(x, \lambda)^2.$$

To see that $a^* > 0$ and $c^* > 0$ for all $\lambda \in (0, \infty)$ we first observe from (5.12) that $4a^*c^* - (b^*)^2 = 4$ requires a^* and c^* to be of the same sign; and this must hold for all $\lambda \in (0, \infty)$ since they are continuous and cannot pass through zero (which would violate (5.12)). Factoring out a^* we have

$$R_1(x, \lambda) = a^*[\theta(x, \lambda)^2 + (b^*/a^*)\theta(x, \lambda)\phi(x, \lambda) + (c^*/a^*)\phi(x, \lambda)^2]$$

with the coefficients of θ^2 and ϕ^2 positive. Therefore R_1 admits a factorization of the form

$$\begin{aligned} R_1(x, \lambda) &= a^*[(\theta(x, \lambda) - \xi\phi(x, \lambda))(\theta(x, \lambda) - \bar{\xi}\phi(x, \lambda))] \\ &= a^*|\theta(x, \lambda) - \xi\phi(x, \lambda)|^2, \end{aligned} \quad (5.13)$$

where $\xi = \xi_1 + i\xi_2$ must satisfy (by (5.12))

$$\xi_1 = -b^*/(2a^*) \text{ and } \xi_2^2 = (c^*/a^*) - [(b^*)^2/(4(a^*)^2)] = 1/(a^*)^2. \quad (5.14)$$

Since a^* , b^* , and c^* are real, we must have either $\xi_2 = 1/a^*$ or $\xi_2 = -1/a^*$; but either way the factorization remains the same with ξ and $\bar{\xi}$ switched. Since $|\theta - \xi\phi|^2 > 0$, it follows from the above factorization that $a^*(\lambda) > 0$ for all $\lambda \in (0, \infty)$; otherwise, $\lim_{x \rightarrow \infty} R_1(x, \lambda) \leq 0$ contradicting the fact that $R_1(\infty, \lambda) = 1/\sqrt{\lambda} > 0$. Hence, also $c^*(\lambda) > 0$ for all $\lambda \in (0, \infty)$. ■

Since the definition of ξ_2 must be $\pm 1/a^*(\lambda)$ from (5.14) and since this indeterminacy is actually immaterial, we choose to take $\xi_2 = 1/a^*(\lambda)$, so that

$$\xi(\lambda) := -\frac{b^*}{2a^*} + i \frac{1}{a^*}. \quad (5.15)$$

Using the Frobenius solutions normalized by (2.16) we now define the complex-valued solution of (5.1) for real $\lambda \in (0, \infty)$, by

$$\psi(x, \lambda) := \theta(x, \lambda) - \xi(\lambda)\phi(x, \lambda). \quad (5.16)$$

We now prove the following lemma that equation (5.1) satisfies *Condition A* for all $\lambda \in (0, \infty)$.

LEMMA 4*. Assume $q(x)$ satisfies **Assumption 1, Case I**, and **Assumptions 2, 3**. Then for $x_0 > 0$ and all $\lambda \in (0, \infty)$

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \psi(x, \lambda)^2 dx}{\int_{x_0}^N |\psi(x, \lambda)|^2 dx} = 0. \quad (5.17)$$

PROOF: Since equation (4.13) is satisfied by all linear combinations of $\phi(\cdot, \lambda)^2$, $\theta(\cdot, \lambda)\phi(\cdot, \lambda)$ and $\theta(\cdot, \lambda)^2$ (see [2, Lemma 1, p. 6584]), it follows that $\psi(\cdot, \lambda)^2$ is a solution of (4.13) and since it is complex-valued, also that $\text{Re}[\psi(\cdot, \lambda)^2]$ and $\text{Im}[\psi(\cdot, \lambda)^2]$ satisfy (4.13). Accordingly, it follows that there exist solutions $U_2 = (P_2, Q_2, \text{Re}(\psi^2))^T$ and $U_3 = (P_3, Q_3, \text{Im}(\psi^2))^T$ of the first order system (1.6), since any real solution R of (4.13) can be used to generate a solution of (1.6) having R as its third component; e.g., let $Q' = -R'$ and $P = -Q'/2 - (\lambda - q)R$. From (5.13) and (5.16) we readily deduce the following representations of $R_1(\cdot, \lambda)$, $\text{Re}[\psi(\cdot, \lambda)]^2$, and $\text{Im}[\psi(\cdot, \lambda)]^2$ of the form (5.11) (or, the third component of (5.11)):

$$\begin{aligned} R_1(x, \lambda) &= a^*\theta^2 - 2a^*\xi_1\theta\phi + a^*(\xi_1^2 + \xi_2^2)\phi^2 \\ \text{Re}[\psi(x, \lambda)]^2 &= \theta^2 - 2\xi_1\theta\phi + (\xi_1^2 - \xi_2^2)\phi^2 \\ \text{Im}[\psi(x, \lambda)]^2 &= -2\xi_2\theta\phi + 2\xi_1\xi_2\phi^2. \end{aligned}$$

It now follows from these formulas that the above solutions U_2 and U_3 associated with $\text{Re}[\psi(\cdot, \lambda)]^2$ and $\text{Im}[\psi(\cdot, \lambda)]^2$ are orthogonal to U_1 in the sense of the inner product defined in (3.7), i.e., we have

$$\langle U_1, U_2 \rangle = 2[a^*(\xi_1^2 - \xi_2^2) + a^*(\xi_1^2 + \xi_2^2)] - 4a^*\xi_1^2 = 0,$$

and

$$\langle U_1, U_3 \rangle = 2[a^*(2\xi_1\xi_2) + 0] - 4a^*\xi_1\xi_2 = 0.$$

Hence it follows from Lemma 3(i) that for all $x_0 > 0$

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \text{Re}[\psi(x, \lambda)]^2 dx}{\int_{x_0}^N R_1(x, \lambda) dx} = 0$$

and

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \text{Im}[\psi(x, \lambda)]^2 dx}{\int_{x_0}^N R_1(x, \lambda) dx} = 0,$$

from which (5.17) follows. \blacksquare

LEMMA 5* (*Al-Naggar and Pearson*). We assume for equation (5.1) that **Assumption 1, Case I**, and **Assumptions 2,3** hold. Let $I \subset (-\infty, \infty)$ be an interval on which Condition A holds. Then
(i) There exists a complex valued function $M(\lambda)$ on I which is uniquely defined by the properties:

$$(a) \quad \text{Im}[M(\lambda)] > 0 \quad \text{and} \quad (b) \quad \lim_{N \rightarrow \infty} \frac{\int_{x_0}^N (\theta(x, \lambda) - M(\lambda)\phi(x, \lambda))^2 dx}{\int_{x_0}^N |\theta(x, \lambda) - M(\lambda)\phi(x, \lambda)|^2 dx} = 0, \quad \text{for all } x_0 > 0.$$

where $\{\phi(\cdot, \lambda), \theta(\cdot, \lambda)\}$ are the Frobenius solutions defined in (2.16).

PROOF: The proof is the same as that for Lemma 1 in [1]. The proof of this lemma does not depend in any essential way on the choice of the fundamental system of equation (5.1). \blacksquare

Unfortunately, the corresponding statement (ii) from Lemma 5 does not carry over immediately to the doubly singular problem (5.1)-(5.2) by borrowing information from [1]; particularly, the proof of Theorem 2 in [1] makes use of asymptotic behaviour of solutions which are fixed by initial conditions at a regular left endpoint, and therefore do not apply to the Frobenius solutions $\{\phi, \theta\}$. The Titchmarsh-Weyl m -function (5.6) was first introduced in the papers [16, 10, 14]: and it wasn't discovered to be a generalized Nevanlinna function in the **LP** case at $x = 0$ until the 2010 paper [14]. A direct generalization of Theorem 2 of [1] for cases when the left endpoint is singular remains unknown. However, we can recover the analogue of part (ii) of Lemma 5 by making appeal to the uniqueness result in Lemma 5*(i) and glean information on the boundary behaviour of $m(z)$ from known information on the boundary behaviour of $m_A(z)$. This is the objective of Lemma 6*. To this end, it will be helpful to introduce notation for the boundary values of the “regular” and “doubly singular” Titchmarsh-Weyl functions $m_A(\lambda)$ and $m(\lambda)$ and for the corresponding Ψ -functions defined in (4.6) and (5.6).

Definition. Associated with the m -functions, $m_A(\lambda)$ and $m(\lambda)$, for the problem with regular left endpoint and for the doubly singular problem, respectively, we define for all $x \in (0, \infty)$ and all $\lambda \in (0, \infty)$:

$$m_A^+(\lambda) := \lim_{\epsilon \downarrow 0} m_A(\lambda + i\epsilon), \quad (5.18)$$

$$\Psi_A^+(x, \lambda) := \lim_{\epsilon \downarrow 0} \Psi_A(\lambda + i\epsilon) = u(x, \lambda) + m_A^+(\lambda)v(x, \lambda), \quad (5.19)$$

$$m^+(\lambda) := \lim_{\epsilon \downarrow 0} m(\lambda + i\epsilon), \quad (5.20)$$

$$\Psi^+(x, \lambda) := \lim_{\epsilon \downarrow 0} \Psi(\lambda + i\epsilon) = \theta(x, \lambda) - m^+(\lambda)\phi(x, \lambda), \quad (5.21)$$

LEMMA 6*. We assume for equation (5.1) that **Assumption 1, Case I**, and **Assumptions 2,3** hold. Then

(i) for all $x \in (0, \infty)$ and all z with $\text{Im } z \neq 0$

$$\Psi(x, \lambda) = \frac{\Psi_A(x, z)}{-\phi'(A, z) + m_A(z)\phi(A, z)}. \quad (5.22)$$

(ii) For all $x \in (0, \infty)$ and all $\lambda \in (0, \infty)$

$$\Psi^+(x, \lambda) = \frac{\Psi_A^+(x, \lambda)}{-\phi'(A, \lambda) + m_A^+(\lambda)\phi(A, \lambda)}. \quad (5.23)$$

(iii) For $x_0 > 0$ and all $\lambda \in (0, \infty)$

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \Psi^+(x, \lambda)^2 dx}{\int_{x_0}^N |\Psi^+(x, \lambda)|^2 dx} = 0. \quad (5.24)$$

(iv) For all $\lambda \in (0, \infty)$

$$\operatorname{Im} m_+(\lambda) = \frac{\operatorname{Im} m_A^+(\lambda)}{|m_A^+(\lambda)\phi(A, \lambda) - \phi'(A, \lambda)|^2} > 0. \quad (5.25)$$

(v) For all $\lambda \in (0, \infty)$ the complex valued function $\xi(\lambda)$ defined in (5.15) is the boundary value of the Titchmarsh-Weyl m-function, that is,

$$\xi(\lambda) = \lim_{\epsilon \downarrow 0} m(\lambda + i\epsilon). \quad (5.26)$$

PROOF. For (i) make use of the fact that for $\operatorname{Im} z \neq 0$ both $\Psi_A(x, z) = u(x, \lambda) + m_A(\lambda)v(x, \lambda)$ and $\Psi(x, z) = \theta(x, \lambda) - m(\lambda)\phi(x, \lambda)$ are in $L_2(x_0, \infty)$, and therefore linearly dependent. Using $W_x(\phi, \theta) = W_x(\phi, \Psi) = 1$, the relation of linear dependence is found to be

$$\Psi(x, z) = \frac{\Psi_A(x, z)}{W_x(\phi, u + m_A(v))},$$

and (5.22) follows on evaluation of the denominator at $x = A$ making use of the initial conditions (3.1). For (ii) put $z = \lambda + i\epsilon$ in (5.22) and pass $\epsilon \rightarrow 0$. For (iii) put (5.23) into (5.24) and factor the constant terms out of the integrals to get the equivalent statement

$$\lim_{N \rightarrow \infty} \frac{\int_{x_0}^N \Psi_A^+(x, \lambda)^2 dx}{\int_{x_0}^N |\Psi_A^+(x, \lambda)|^2 dx} = 0.$$

But $\Psi_A^+(x, \lambda)$ is known to satisfy *Condition A* by Lemma 5(ii), Lemma 6, and Lemma 4 with (i.e. by Theorem 2 of [1] applied to the problem (4.1)-(4.2)). Hence it follows that (5.24) also holds for all $\lambda \in (0, \infty)$ and all $x_0 > 0$; in other words, $\Psi^+(x, \lambda)$ also satisfies *Condition A*. For (iv) use

$$m^+(\lambda) = W_x(\theta(\cdot, \lambda), \Psi^+(\cdot, \lambda))$$

and substitute the right hand side of (5.23) for $\Psi^+(x, \lambda)$, evaluating $W_x(\theta, u)$ and $W_x(\phi, v)$ at $x = A$ using the initial conditions (3.1), to obtain for all $\lambda \in (0, \infty)$

$$m^+(\lambda) = \frac{\theta(A, \lambda)m_A^+(\lambda) - \theta'(A, \lambda)}{\phi(A, \lambda)m_A^+(\lambda) - \phi'(A, \lambda)}.$$

Then (5.25) follows by taking imaginary parts on both sides. The right hand side of (5.25) is positive for all $\lambda \in (0, \infty)$ because the numerator is positive by Theorem 1 (equation (4.28)), and the denominator never becomes zero (by separating real and imaginary parts and observing that the cases $\phi(A, \lambda) = 0$ and $\phi(A, \lambda) \neq 0$ both yield a positive denominator). To prove (v) we observe first that for all $\lambda \in (0, \infty)$, $m^+(\lambda)$ has positive imaginary part (by (5.25)) and $\Psi^+(x, \lambda)$ satisfies (by (5.24)) property (b) in Lemma 5*(i). Similarly, the function ξ defined in (5.15) has positive imaginary part (see Lemma 3(ii)) for all $\lambda \in (0, \infty)$ and the solution $\psi(x, \lambda)$ defined in (5.16) satisfies (see Lemma 4*) property (b) in Lemma 5*(i). Hence by the uniqueness of the function $M(\lambda)$ satisfying the two properties of Lemma 5*(i), the functions $m^+(\lambda)$ and $\xi(\lambda)$ must be identical, that is, (5.26) holds. ■

We are now ready to prove the representation of $f(\lambda)$ in the form (1.5). This represents the “doubly singular” analogue of the spectral density function characterization of **Theorem 1**.

Theorem 3 We assume that **Assumption 1, Case I**, and **Assumptions 2,3** hold. Let $\xi(\lambda)$ be defined as in (5.15) and $\psi(\cdot, \lambda)$ as in (5.16). Then the spectral function defined by (5.8) for the problem (5.1)-(5.2) (in both the **LC** and **LP** cases at $x = 0$) is absolutely continuous for $\lambda \in (0, \infty)$ and the

corresponding spectral density function admits the following representations for $\lambda \in (0, \infty)$:

$$f(\lambda) := \rho'(\lambda) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \text{Im}[m(\lambda + i\epsilon)] \quad (5.27)$$

$$= \frac{\xi_2(\lambda)}{\pi} \quad (5.28)$$

$$= \frac{1}{\pi a^*(\lambda)} \quad (5.29)$$

$$= \frac{1}{\pi [P_1(x, \lambda)(\phi(x, \lambda))^2 + Q_1(x, \lambda)\phi(x, \lambda)\phi'(x, \lambda) + R_1(x, \lambda)(\phi'(x, \lambda))^2]}. \quad (5.30)$$

PROOF: The statement (5.28), and the absolute continuity of the spectral function ρ , follows from Lemma 6*(v) by taking imaginary parts of each side of (5.26). The statment (5.29) follows from the definition of ξ_2 in (5.15). To obtain (5.30) substitute $U_1 = (P_1, Q_1, R_1)^T$ from the representation (5.11) in terms of $\{\theta(x, \lambda), \phi(x, \lambda)\}$ and collect coefficients of $a^*(\lambda)$, $b^*(\lambda)$ and $c^*(\lambda)$ to obtain

$$P(\phi)^2 + Q\phi\phi' + R(\phi')^2 = a^*(\lambda)[W_x(\phi, \theta)]^2 = a^*(\lambda). \quad \blacksquare$$

6 Some Examples with Explicitly Known Spectral Density Functions

In this section we give the explicit formulas from [10, 14] for the Frobenius solution $\phi(\cdot, \lambda)$, the Titchmarsh-Weyl m-function, and the spectral density function for some examples of the special potential (5.5). We restrict attention to those cases which will be used as test problems for the numerical algorithms in Sections 8 and 9.

Example 1: [$q_0 = -a, a > 0; q_1 = \ell(\ell + 1)$] Hydrogen Atom

$$-y'' + \left(-\frac{a}{x} + \frac{\ell(\ell + 1)}{x^2}\right)y = \lambda y \quad a > 0, \quad 0 < x < \infty. \quad (6.1)$$

The first Frobenius solution with normalization (2.9) is

$$\begin{aligned} \phi(x, \lambda) &= x^{\ell+1} \left[1 + \sum_{n=1}^{\infty} a_n(\lambda) x^n \right] \\ &= x^{\ell+1} e^{ix\sqrt{\lambda}} M(\ell + 1 - \beta, 2\ell + 2, -2ix\sqrt{\lambda}) \\ &= \frac{1}{(-2i\sqrt{\lambda})^{\ell+1}} \mathcal{M}_{\beta, \ell+\frac{1}{2}}(-2ix\sqrt{\lambda}), \end{aligned} \quad (6.2)$$

with $\beta := ia/2\sqrt{\lambda}$ for all $\lambda \in \mathbb{C}$. Here M is the confluent hypergeometric function of first kind and \mathcal{M} is the corresponding Whittaker function of first kind. The coefficients $a_n(\lambda)$ are polynomials in λ of degree $[n/2]$ which are generated from the recurrence relation

$$a_n(\lambda) = -\frac{a}{n(n+2\ell+1)} a_{n-1}(\lambda) - \frac{\lambda}{n(n+2\ell+1)} a_{n-2}(\lambda),$$

and the first three are

$$\begin{aligned} a_1 &= -\frac{a}{2\ell+2}, \\ a_2(\lambda) &= \frac{a^2 - 2(\ell+1)\lambda}{2!(2\ell+2)(2\ell+3)}, \\ a_3(\lambda) &= \frac{-a^3 + (6\ell+8)a\lambda}{3!(2\ell+2)(2\ell+3)(2\ell+4)}, \end{aligned}$$

The Titchmarsh-Weyl m-function arising from (5.6) is

$$m_\ell(\lambda) = k_\ell(\lambda) \left[-a \log(-2i\sqrt{\lambda}) - a\Psi(1 - ia/(2\sqrt{\lambda})) - 2\gamma a + i\sqrt{\lambda} \right] + p_\ell(\lambda), \quad (6.3)$$

where Ψ is the psi or digamma function, γ is Euler's constant,

$$k_\ell(\lambda) := \frac{1}{[(2\ell+1)!]^2} \prod_{j=1}^{\ell} (4\lambda j^2 + a^2),$$

and where $p_\ell(\lambda)$ is a polynomial of degree ℓ (see [10, 17]). We take $0 \leq \arg(\lambda) < 2\pi$, so that the branch cut for $\sqrt{\lambda}$ and m_ℓ is on the positive real λ -axis.

The associated spectral density function arising from (5.9) is

$$f_\ell(\lambda) := \lim_{\epsilon \rightarrow 0} \frac{\text{Im}[m_\ell(\lambda + i\epsilon)]}{\pi} = k_\ell(\lambda) \left[\frac{a}{1 - e^{-\pi a/\sqrt{\lambda}}} \right]. \quad (6.4)$$

Example 2: [$q_0 = -a, a < 0; q_1 = \ell(\ell+1)$] Repulsive Coulomb

$$-y'' + \left(-\frac{a}{x} + \frac{\ell(\ell+1)}{x^2} \right) y = \lambda y, \quad a < 0, \quad 0 < x, \infty \quad (6.5)$$

The first Frobenius solution with normalization (2.9) is (same as (6.2) with $a < 0$)

$$\begin{aligned} \phi(x, \lambda) &= x^{\ell+1} \left[1 + \sum_{n=1}^{\infty} a_n(\lambda) x^n \right] \\ &= x^{\ell+1} e^{ix\sqrt{\lambda}} M(\ell+1-\beta, 2\ell+2, -2ix\sqrt{\lambda}) \\ &= \frac{1}{(-2i\sqrt{\lambda})^{\ell+1}} \mathcal{M}_{\beta, \ell+\frac{1}{2}}(-2ix\sqrt{\lambda}), \end{aligned} \quad (6.6)$$

where $\beta := ia/2\sqrt{\lambda}$, and $a < 0$. The recurrence relation and first three coefficients, $a_n(\lambda)$, are the same as in Example 1 with $a < 0$. The Titchmarsh-Weyl m-function arising from (5.6) is

$$m_\ell(\lambda) = k_\ell(\lambda) \left[-a \log(-2i\sqrt{\lambda}) - a\Psi(1 - ia/(2\sqrt{\lambda})) - 2\gamma a + i\sqrt{\lambda} \right] + p_\ell(\lambda). \quad (6.7)$$

where $a < 0$, and $k_\ell(\lambda)$, $p_\ell(\lambda)$ are the same, with $a < 0$, as given above for the hydrogen atom. The branch cut is taken again on the positive real λ -axis.

The associated spectral density function arising from (5.9) is

$$f_\ell(\lambda) = k_\ell(\lambda) \left(\frac{|a|}{\exp(|a|\pi/\sqrt{\lambda}) - 1} \right), \quad (6.8)$$

Example 3: [$q_0 = \nu^2 - 1/4, \nu \neq M/2, M = 0, 1, 2, \dots; q_1 = 0$] Bessel Equation of Non-integer Order

$$-y'' + \frac{\nu^2 - 0.25}{x^2} y = \lambda y, \quad \nu > 0, \nu \neq N/2, N = 1, 2, \dots, \quad (6.9)$$

The first Frobenius solution with normalization (2.6) is

$$\phi(x, \lambda) := x^{\nu+0.5} \left[1 + \sum_{j=1}^{\infty} \frac{(-1)^j \lambda^j x^{2j}}{j!(\nu+1)_j 2^{2j}} \right] = 2^\nu \Gamma(\nu+1) \lambda^{-\nu/2} x^{1/2} J_\nu(\sqrt{\lambda} x) \quad (6.10)$$

The Titchmarsh-Weyl m-function arising from (5.6) is

$$m(\lambda) = -\frac{\pi}{2^{2\nu+1}\Gamma^2(\nu+1) \cdot \sin(\nu\pi)} e^{-i\nu\pi} \lambda^\nu \quad (6.11)$$

where $0 \leq \arg(\lambda) < 2\pi$, so that the branch cut for λ^ν is on the positive real λ -axis.

The associated spectral density function arising from (5.9) is

$$f_\nu(\lambda) = \frac{\lambda^\nu}{2^{2\nu+1}\Gamma^2(\nu+1)}. \quad (6.12)$$

Example 4: $[q_0 = N^2 - 1/4, N = 0, 1, 2, \dots; q_1 = 0]$ Bessel Equation of Integer Order

$$-y'' + \frac{N^2 - 0.25}{x^2} y = \lambda y, \quad a > 0, N = 0, 1, \dots, \quad (6.13)$$

The first Frobenius solution with normalization (2.12) is

$$\phi(x, \lambda) := x^{N+0.5} \left[1 + \sum_{j=1}^{\infty} \frac{(-1)^j \lambda^j x^{2j}}{j!(N+1)_j 2^{2j}} \right] = 2^\nu \Gamma(N+1) \lambda^{-N/2} x^{1/2} J_N(\sqrt{\lambda} x), \quad N = 0, 1, 2, \dots \quad (6.14)$$

The Titchmarsh-Weyl m-function arising from (5.6) is

$$\begin{aligned} m_0(\lambda) &= -\log(-2i\sqrt{\lambda}) + \gamma - 2\ell n 2 \\ m_N(\lambda) &= \frac{\lambda^N}{2^{2N}(N!)^2} m_0(\lambda) + \frac{\lambda^N H_{N+1}}{2^{2N+1}(N!)^2}, \quad N \geq 1. \end{aligned} \quad (6.15)$$

where $0 \leq \arg(\lambda) < 2\pi$, so that the branch cut for m_0 is on the positive real λ -axis.

The associated spectral density function arising from (5.9) is

$$f_N(\lambda) = \frac{\lambda^N}{2^{2N+1}(N!)^2}. \quad (6.16)$$

7 Numerical Methods

In this section and the following two sections we describe some new numerical methods for obtaining approximations to the spectral density function (1.4) and then the spectral function, by making use of the new representation (5.30) in Theorem 3, and compare their performance with **SLEDGE**. For general information and discussion of numerical methods for Sturm-Liouville problems we refer to Pryce's book [21] and for spectral function computation using **SLEDGE** we refer to our previous papers [20, 6, 15].

Many numerical methods for (1.1) break down near a singular point at $x = 0$. However, when we take this singular point to be a regular singular point, it admits a convergent Frobenius expansion, and then a finite number of leading terms in the sum can be used as an initial approximation near $x = 0$. For equation (2.4) the indicial equation is (2.5) and the principal solution is the first Frobenius solution with the larger indicial root,

$$r_1 = \nu := 0.5 + 0.5\sqrt{1 + 4q_0}.$$

This solution has the general form

$$\phi(x, \lambda) = \sum_{n=0}^{\infty} a_n x^{n+\nu}, \quad (7.1)$$

and the general recurrence formula is

$$a_1 = \frac{q_1 a_0}{\nu(\nu+1) - q_0},$$

and for $n > 1$

$$a_n = \frac{-\lambda a_{n-2} + q_1 a_{n-1} + \sum_{k=0}^{n-2} q_{k+2} a_{n-2-k}}{(\nu + n - 1)(\nu + n) - q_0}.$$

The choice for a_0 fixes the normalization of $\phi(\cdot, \lambda)$, and in this paper we have made the simple choice $a_0 = 1$ in all the cases (2.6), (2.9) and (2.12); this ensures that the properties **(i)**, **(ii)**, **(iii)** of section 2 hold in all the cases of **Assumption 1**.

We note that there is a risk of loss of significance in the computation of $a_n(\lambda)$ for very large λ , because for moderate n the powers of λ in the numerator of a_n build up faster than the denominator does. We have found that keeping

$$x < x_0(\lambda) := |q_0|/\sqrt{\lambda} \quad (7.2)$$

and using the truncated Frobenius series (to full machine precision) only on $(0, x_0(\lambda)]$ works well. For $x > x_0(\lambda)$ we use the methods from [12] and [13] for regular problems. In brief, the algorithm is as follows:

- (i)** For a given λ choose a ‘matching point’ $x(\lambda)$.
- (ii)** Use the first Frobenius solution (7.1) (this is the principal solution near zero) on the interval $(0, x_0(\lambda)]$ to produce values for solution and its derivative (usually to machine precision) at $x_0(\lambda)$.
- (iii)** Apply standard methods to numerically estimate y for (5.1) on the interval $[x_0(\lambda), x(\lambda)]$ satisfying initial conditions from **(i)**. Because of the oscillation in y for $\lambda > 0$, we use a piecewise trigonometric approximation to y .
- (iv)** Approximate the solution $P(x, \lambda)$, $Q(x, \lambda)$, and $R(x, \lambda)$ of the initial value problem (1.6)-(1.7) at the matching point $x(\lambda)$ using one of the approaches described below.
- (v)** Substitute the estimates from **(iii)**, **(iv)** into

$$f_x(\lambda) := \frac{1}{\pi [P(x, \lambda)y(x, \lambda)^2 + Q(x, \lambda)y(x, \lambda)y'(x, \lambda) + R(x, \lambda)y'(x, \lambda)^2]}, \quad (7.3)$$

to produce an approximation to the exact spectral density, $f(\lambda)$, given in Theorem 3, equation (5.30).

The two papers [12] and [13] derive two very different approaches to the numerical computation of $(P(b, \lambda), Q(b, \lambda), \text{ and } R(b, \lambda))$. In [12] we constructed a family of recurrence formulas that generated successively more accurate approximations to P , Q , and R and hence to $f(\lambda)$. For fixed $x > 0$ define for each positive integer j the family of functions

$$F_x^j(\lambda) := \frac{1}{\pi [P_j y^2 + Q_j y y' + R_j y'^2]}. \quad (7.4)$$

From [11] for $j = 1$ we define

$$P_1 := \sqrt{\lambda}, \quad Q_1 := 0, \quad R_1 := 1/\sqrt{\lambda}. \quad (7.5)$$

From [12] the next formula in the family for $j = 2$ is defined by

$$P_2 := \sqrt{\lambda - q(x)}, \quad Q_2 := -q'(x)/[2(\lambda - q(x))^{3/2}], \quad R_2 := 1/\sqrt{\lambda - q(x)}. \quad (7.6)$$

The final member that we use is $j = 3$, also defined in [12] as:

$$\begin{aligned} P_3 &:= P_2 + 0.25\gamma_2 + 0.125\gamma_1^2/\gamma_0 \\ Q_3 &:= Q_2 - \frac{d}{dx} \{-0.25\gamma_0^2\gamma_2 + 0.125\gamma_0\gamma_2^2\} \\ R_3 &:= R_2 - 0.25\gamma_2 + 0.125\gamma_0\gamma_1^2 \end{aligned} \quad (7.7)$$

where

$$\gamma_k := \frac{d^k}{dx^k} \left[\frac{1}{\sqrt{\lambda - q(x)}} \right]$$

for $k = 0, 1, 2$. For regular problems on $[A, \infty)$, $A > 0$, it is shown in [12] that each member of this family converges to the spectral function $f_A(\lambda)$ as $x \rightarrow \infty$. For the hydrogen atom potential (6.1) on $[A, \infty)$ the theory of [12] implies that

$$f_A(\lambda) - F_x^j(\lambda) = O(1/x^{2j-1}) \text{ as } x \rightarrow \infty. \quad (7.8)$$

This method requires knowledge of derivatives of the potential $q(x)$.

In [13] we constructed explicit approximations to the solutions of (1.6) with known residual terms that arise during the construction; in particular, replace $P(x, \lambda)$, $Q(x, \lambda)$, and $R(x, \lambda)$ with estimates of the form

$$\begin{aligned} P_N(x) &:= \sqrt{\lambda} + \sum_{j=1}^N a_j/x^j \\ Q_N(x) &:= \sum_{j=1}^N b_j/x^{j+1} \\ R_N(x) &:= 1/\sqrt{\lambda} + \sum_{j=1}^N c_j/x^j, \end{aligned} \quad (7.9)$$

where $\{a_j\}$, $\{b_j\}$, and $\{c_j\}$ will depend on λ but not x . The resulting sums are substituted into (1.6) and the coefficients chosen to match terms of like powers. Then we put the computed coefficients into (7.9) and define the family of approximations

$$f_x^N(\lambda) := \frac{1}{\pi[P_N(x, \lambda)y(x, \lambda)^2 + Q_N(x, \lambda)y(x, \lambda)y'(x, \lambda) + R_N(x, \lambda)y'(x, \lambda)^2]}. \quad (7.10)$$

Specifically, the N th residuals are defined as

$$\begin{pmatrix} \phi_N^P \\ \phi_N^Q \\ \phi_N^R \end{pmatrix} := \begin{pmatrix} P'_N \\ Q'_N \\ R'_N \end{pmatrix} - \begin{pmatrix} 0 & \lambda - q & 0 \\ -2 & 0 & 2(\lambda - q) \\ 0 & -1 & 0 \end{pmatrix} \cdot \begin{pmatrix} P_N \\ Q_N \\ R_N \end{pmatrix}$$

and we attempt to make these small, as $x \rightarrow \infty$, by the choice of coefficients in (7.9). All potentials in the examples of the previous section have the form (5.5), that is,

$$q(x) = A/x + B/x^2, \quad (7.11)$$

where $A = q_1$ and $B = q_0$ and (2.2) is satisfied. It is straightforward to show that

$$\begin{aligned} \phi_N^P &= \left[\sum_{j=1}^N \frac{-ja_j - \lambda b_j + Ab_{j-1} + Bb_{j-2}}{x^{j+1}} \right] + \frac{Bb_{N-1} + Ab_N}{x^{N+2}} + \frac{Bb_N}{x^{N+3}} \\ \phi_N^Q &= \left[\sum_{j=1}^N \frac{-(j-1)b_{j-2} + 2a_j - 2\lambda c_j + 2Ac_{j-1} + 2Bc_{j-2}}{x^j} + \frac{2A + 2B/x}{x\sqrt{\lambda}} \right] \\ &\quad - \frac{Nb_{N-1} + 2Ac_N + 2Bc_{N-1}}{x^{N+1}} + \frac{2Bc_N - (N+1)b_N}{x^{N+2}} \\ \phi_N^R &= \sum_{j=1}^N \frac{-jc_j + b_j}{x^{j+1}}. \end{aligned}$$

If we require the coefficients to satisfy

$$ja_j + \lambda b_j = Ab_{j-1} + Bb_{j-2} \quad (7.12)$$

$$a_j - \lambda c_j = (j-1)b_{j-2}/2 - Ac_{j-1} - Bc_{j-2} + [A\delta_{j1} + B\delta_{j2}]/\sqrt{\lambda} \quad (7.13)$$

$$b_j - jc_j = 0, \quad (7.14)$$

for $j = 1, 2, \dots, N$, then the residuals simplify to

$$\phi_N^P = \frac{Ab_N + Bb_{N-1}}{x^{N+2}} + \frac{Bb_N}{x^{N+3}} \quad (7.15)$$

$$\phi_N^Q = \frac{-Nb_{N-1} + 2Ac_N + 2Bc_{N-1}}{x^{N+1}} + \frac{2Bc_N - (N+1)b_N}{x^{N+2}} \quad (7.16)$$

$$\phi_N^R = 0. \quad (7.17)$$

If we adopt the convention that coefficients with nonpositive subscripts have zero values, then the solution of (7.12)–(7.14) can be written, for $1 \leq j \leq N$,

$$\begin{aligned} a_j &= (t_1 + t_2)/2 \\ c_j &= (t_1 - t_2)/(2\lambda) \\ b_j &= jc_j, \end{aligned}$$

where

$$t_1 = [(Ab_{j-1} + Bb_{j-2})/j$$

and

$$t_2 = 0.5(j-1)b_{j-2} - Ac_{j-1} - Bc_{j-2} - [A\delta_{j1} + B\delta_{j2}]/\sqrt{\lambda}.$$

Since the derivatives of the residuals do not change sign once x is sufficiently large, the theory of [12] implies for that

$$f(\lambda) - f_x^N(\lambda) = O(1/x^{N+1}) \quad (7.18)$$

as $x \rightarrow \infty$.

To numerically estimate the spectral density function $f(\lambda)$, we would usually use the methods (7.4) from [12] because they require knowledge of only the first few derivatives of $q(x)$. But when q has the required special forms, the method (7.10) from [13], often more efficient, can also be used.

8 Numerical Estimation of the Spectral Density Function $f(\lambda)$

In this section we test our implementation of the various numerical methods from the previous section on the examples listed in section 6, for which exact formulas are known for the spectral density function. Then we also test a more interesting example from quantum chemistry for which exact formulas are not known.

For the hydrogen atom potential, Example 1 (equation (6.1)) with $a = 1$, Table 8.1 has numerical output when $\ell = 1$ for many λ with the methods F_x^1 , F_x^2 , F_x^3 , and f_x^6 using the notation of the previous section. Table 8.2 shows the analogous data when $\ell = 2$. Shown are only the errors: absolute when the answer is less than one and relative otherwise. A tolerance of 10^{-14} was used for the numerical integration of the initial value problem for (6.1), starting at $x_0(\lambda)$ from (7.2). Consequently, table entries this small represent errors in y as well as errors due to finite x . Note that for a fixed accuracy, generally larger matching points x are needed when λ is smaller. As expected, the higher order methods F^3 and f^6 are much superior.

Table 8.1. Numerical Error: H Atom ($\ell = 1$) $q(x) = -1/x + 2/x^2$.

λ	$x = x(\lambda)$	F_x^1	F_x^2	F_x^3	f_x^6
0.1	320.0	4.60(-4)	-2.10(-8)	5.62(-12)	2.13(-14)
0.2	225.0	2.19(-5)	-1.18(-9)	4.28(-13)	4.48(-14)
0.4	160.0	5.08(-4)	-2.34(-8)	6.36(-12)	4.56(-15)
1	100.0	5.53(-4)	-2.62(-8)	7.49(-12)	1.25(-13)
2	71.0	9.52(-4)	-4.39(-8)	1.21(-11)	9.60(-14)
4	50.0	-2.55(-4)	1.22(-8)	-2.95(-12)	4.89(-13)
10	32.0	1.41(-3)	-5.93(-8)	1.48(-11)	3.25(-13)
20	22.5	-2.79(-4)	1.14(-8)	-1.81(-12)	7.83(-13)
40	16.0	3.52(-4)	-1.21(-8)	2.91(-12)	8.16(-13)
100	10.0	-3.39(-4)	8.44(-9)	2.52(-13)	2.61(-13)
200	7.0	2.32(-4)	-2.34(-9)	-1.91(-12)	3.02(-13)
400	5.0	-1.04(-4)	-1.66(-9)	2.78(-12)	2.60(-13)
1000	3.2	-4.06(-6)	-6.53(-10)	7.80(-13)	2.82(-13)
2000	2.2	5.84(-6)	5.12(-9)	-2.91(-12)	2.86(-13)
4000	1.6	3.49(-6)	-1.79(-9)	1.34(-12)	2.84(-13)
10000	1.0	2.67(-5)	-6.60(-9)	3.81(-12)	2.95(-13)

Table 8.2. Numerical Error: H Atom ($\ell = 2$) $q(x) = -1/x + 6/x^2$.

λ	$x = x(\lambda)$	F_x^1	F_x^2	F_x^3	f_x^6
0.1	320.0	-3.13(-6)	1.35(-10)	-3.45(-14)	3.95(-15)
0.2	225.0	-4.79(-6)	2.13(-10)	-5.60(-14)	2.98(-15)
0.4	160.0	-4.28(-6)	1.83(-10)	-4.54(-14)	3.00(-15)
1	100.0	-2.82(-5)	1.20(-9)	-2.98(-13)	8.32(-15)
2	71.0	-7.24(-5)	2.87(-9)	-6.41(-13)	1.92(-14)
4	50.0	8.09(-5)	-2.97(-9)	5.83(-13)	5.28(-15)
10	32.0	-8.59(-4)	2.24(-8)	-7.48(-13)	1.69(-13)
20	22.5	2.80(-4)	-3.67(-9)	-1.75(-12)	8.68(-13)
40	16.0	-2.36(-4)	-2.06(-9)	4.70(-12)	6.52(-14)
100	10.0	1.69(-4)	1.66(-8)	-1.22(-11)	8.75(-14)
200	7.0	-4.57(-5)	-2.62(-8)	1.71(-11)	3.02(-14)
400	5.0	-3.42(-5)	2.25(-8)	-1.26(-11)	-5.91(-14)
1000	3.2	-8.80(-6)	2.46(-9)	-6.75(-13)	8.21(-13)
2000	2.2	1.06(-4)	-2.25(-8)	1.24(-11)	8.62(-13)
4000	1.6	-2.78(-5)	5.40(-9)	-2.15(-12)	8.09(-13)
10000	1.0	-1.42(-4)	2.38(-8)	-1.17(-11)	8.94(-13)

The next choice is the Bessel Equation, Example 3 (equation (6.9)), with $\nu = 1/3$:

$$q(x) = -5/(36x^2). \quad (8.1)$$

The error behavior is similar to that in the previous tables.

Table 8.3. Numerical Error: $q(x) = -5/(36x^2)$

λ	$x = x(\lambda)$	F_x^1	F_x^2	F_x^3	f_x^6
0.1	320.0	-3.26(-7)	4.61(-11)	3.21(-14)	5.37(-14)
0.2	225.0	1.22(-6)	-1.13(-10)	1.59(-13)	6.86(-14)
0.4	160.0	-5.18(-7)	7.31(-11)	4.90(-14)	8.34(-14)
1	100.0	2.34(-6)	-3.48(-10)	2.85(-13)	1.12(-13)
2	71.0	3.30(-6)	-4.93(-10)	3.92(-13)	1.47(-13)
4	50.0	3.71(-6)	-5.53(-10)	4.38(-13)	1.63(-13)
10	32.0	-1.51(-6)	2.14(-10)	1.49(-13)	2.49(-13)
20	22.5	5.26(-6)	-7.86(-10)	6.76(-13)	2.85(-13)
40	16.0	-1.78(-6)	2.51(-10)	1.58(-13)	2.76(-13)
100	10.0	5.92(-6)	-8.26(-10)	7.22(-13)	2.83(-13)
200	7.0	-5.92(-6)	9.12(-10)	-1.74(-13)	2.95(-13)
400	5.0	5.92(-6)	-8.82(-10)	7.36(-13)	2.97(-13)
1000	3.2	-1.78(-6)	2.51(-10)	1.54(-13)	2.72(-13)
2000	2.2	-5.78(-6)	8.89(-10)	-1.65(-13)	2.91(-13)
4000	1.6	-1.78(-6)	2.51(-10)	1.70(-13)	2.88(-13)
10000	1.0	5.92(-6)	-8.82(-10)	5.98(-12)	2.63(-13)

In the papers of Bain et al [4], Brändas et al [5], and Engdahl et al [7], [8], [9] can be found a potential with a “barrier” near $x = 2$ and decaying rapidly to zero as $x \rightarrow \infty$:

$$q(x) = \frac{\ell(\ell+1)}{x^2} - \frac{a}{x} + 15x^2e^{-x}. \quad (8.2)$$

For this example we have $q_0 = \ell(\ell+1)$, $q_1 = -a$, $q_2 = q_3 = 0$, and for $k \geq 2$

$$q_{k+2} = (-1)^k \frac{15}{(k-2)!}.$$

For $a = 1$, Table 8.4 displays the results for several values of x to show the rapid convergence as $x \rightarrow \infty$. A tolerance of 10^{-14} was used for the numerical integration of y .

Table 8.4. F_x^3 Estimates for Barrier Potential (8.2) with $a = 1$.

x	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 0$	$\ell = 1$	$\ell = 2$
$\lambda = 7$			$\lambda = 10$			
5.	0.142809355	0.019804657	0.0004166628	1.686525464	1.728228916	0.1242771047
10.	0.142828980	0.019801387	0.0004162081	1.686646374	1.728086680	0.1242724151
15.	0.142829143	0.019801395	0.0004162075	1.686647533	1.728085796	0.1242722883
20.	0.142829149	0.019801396	0.0004162075	1.686647559	1.728085772	0.1242723271
25.	0.142829149	0.019801396	0.0004162075	1.686647559	1.728085772	0.1242723271
$\lambda = 20$			$\lambda = 40$			
5.	1.999374819	4.314112367	2.8784054457	2.558971562	11.31991454	17.270757428
10.	1.999374881	4.314112204	2.8784044730	2.558971266	11.31991563	17.270756351
15.	1.999374882	4.314112311	2.8784043230	2.558971293	11.31991552	17.270756523
20.	1.999374882	4.314112307	2.8784043239	2.558971293	11.31991552	17.270756528
25.	1.999374882	4.314112307	2.8784043240	2.558971293	11.31991552	17.270756528

9 Numerical Estimation of the Spectral Function $\rho(\lambda)$

Associated with the density function $f(\lambda)$ is the associated spectral function defined by

$$\rho(\lambda) := \int_0^\lambda f(\mu) d\mu. \quad (9.1)$$

In [11] for problems regular at $x = 0$ we estimated ρ using F^1 and compared with the package SLEDGE [20, 15]; generally the $\rho(\lambda)$ computation using a quadrature routine for (9.1) and the F^1 formula ran considerably faster than SLEDGE, but still had the drawback that rather large x -intervals were required for the F^1 calculation. Here we apply the methods of this paper for computing ρ by estimating f in (9.1), and performing a quadrature, to the examples in section 6 for which exact answers are known, and again compare with SLEDGE.

The SLEDGE software for estimating $\rho(\lambda)$ is based on the Levitan-Levinson characterization of the spectral function as a limit of step spectral functions over a finite interval approximation (second formula in (5.8)); this is a totally different approach than the present approach of this paper which relies on the family of F^j -approximants, together with the quadrature in (9.1). For the case of two singular endpoints, the performance of SLEDGE for computing the spectral function on examples having explicit formulas for the spectral function was reported on in [15]. As reported there, one of the major weaknesses of the SLEDGE package is obtaining high accuracy in the $\rho(\lambda)$ calculation when λ is large; this is due primarily to the fact that SLEDGE does not rely on asymptotic approximations for the eigenvalues and eigenfunction norm reciprocals, but computes them numerically as required for implementing the $\rho_b(\lambda)$ -formula in (5.8). Experience in using SLEDGE on doubly singular problems is that very large computing times are required due to the computation of large numbers of eigenvalue - eigenfunction norm pairs, and that there is significant loss of accuracy when λ becomes sufficiently large. As the timing and accuracy data of this section shows, doubly singular problems can be handled with high accuracy and much reduced computing times by making use of the F_x^j -approximants and the f_x^N -approximants of this paper, along with the quadratures for computing $\rho(\lambda)$ in (9.1); this represents a major improvement in computational technique over the SLEDGE algorithm for spectral function computation.

Following SLEDGE, we assume approximations are sought for a finite set of λ -values in the continuous spectrum, $(0, \infty)$, ordered so that

$$0 < \lambda_1 < \lambda_2 < \dots < \lambda_m.$$

Then with $\rho(0)$ given (or computed via SLEDGE) we estimate

$$\rho(\lambda_1) = \rho(0) + \int_0^{\lambda_1} f(\mu) d\mu$$

and for $j = 2, 3, \dots, m$

$$\rho(\lambda_j) = \rho(\lambda_{j-1}) + \int_{\lambda_{j-1}}^{\lambda_j} f(\mu) d\mu \quad (9.2)$$

using an adaptive quadrature code with f replaced by F_x^j or f_x^N approximations. Here we report some timing and accuracy data for the four examples listed in section 6.

The spectral functions on $(0, \infty)$ for these examples are known in closed form by putting the exact spectral density functions from (6.4), (6.8), (6.12), and (6.16) into (9.1) and performing an exact integration. The resulting closed form formulas for $\rho(\lambda)$ were used for the four examples to compare with the numerical approximations and to generate the ‘exact’ error; the errors are taken as absolute if the exact value of $\rho(\lambda)$ is less than one, and relative otherwise.

For the Bessel equation of order 1, Example 4 (equation (6.13 with $N=1$), we used $N = 7$ in the approximation (7.10) (that is, the scheme from [13, Sec 4]). Output data for six λ -values is displayed in Table 9.1. The quadrature tolerance was 10^{-8} and the tolerance for the initial value problem was 10^{-9} . Note that, at this tolerance, all the apparent error arises from the first integration interval and is passed on through the sum in (9.2).

Table 9.1. $\rho(\lambda)$ for the first order Bessel equation on $(0, \infty)$ ($q(x) = 0.75/x^2$)

x	$\lambda = 1$	$\lambda = 2$	$\lambda = 4$	$\lambda = 10$	$\lambda = 20$	$\lambda = 40$
6.	0.06318042	0.25068042	1.00068041	6.25068041	25.00068041	100.00068041
12.	0.06254252	0.25004252	1.00004252	6.25005252	25.00004252	100.00004252
24.	0.06250266	0.25000266	1.00000266	6.25000266	25.00000266	100.00000266
36.	0.06250000	0.25000000	1.00000000	6.25000000	25.00000000	100.00000000

The data for estimating $f(\lambda)$ in section 8 showed that as λ gets larger, smaller values of the matching point $x = x(\lambda)$ are needed for a given accuracy. The data in Table 9.1 for ρ exhibit this phenomena. Hence, from efficiency considerations in order to compute $\rho(\lambda)$ we want the choice of matching point x to vary with the integer N , or even better, pointwise with λ . For $q(x) = 0.75/x^2$ it can be shown that the absolute error in $f(\lambda)$ for a given N is proportional to

$$\frac{1}{x^{N+2}\lambda^{N-1/2}}.$$

This suggests that taking $x \sim 1/\lambda^{(2N-1)/(2N+4)}$ would be a good heuristic for the matching point. Similarly, for the family of approximants, F^N , from (7.4)–(7.7) the corresponding form for the absolute error in $f(\lambda)$ is

$$\frac{1}{x^{2N}\lambda^{N-1/2}},$$

so that $x \sim 1/\lambda^{(2N-1)/(4N)}$ would be an appropriate matching point. The latter is roughly $1/\sqrt{\lambda}$. As mentioned earlier, these formulas would change for a different q . Also, the heuristic would differ for relative errors. A similar analysis for the general potential $q(x) = A/x + B/x^2$ suggests a good first value of matching point would be

$$x = x(\lambda) := |A|/(2\lambda) + \sqrt{A^2/(4\lambda^2) + |B|/\lambda}. \quad (9.3)$$

We have written a research code, called AutoB, for which the only inputs required are the set of λ points, the $\rho(0)$ value, and the accuracy desired. If q has the form of (7.11) or the form of similar potentials in [13], then we use the appropriate f_x^N formula in (7.10) with N chosen to be a function of the accuracy sought. Otherwise, we use F^3 from (7.4) which requires knowledge of derivatives of q . We report the performance of AutoB on the four examples in section 6 using (9.3) as the initial choice of matching point. Given a prescribed tolerance τ , for each λ the matching point x is then increased until

$$|\text{error estimate}| \leq \max\{1, |\text{output value}|\} \tau$$

holds. Estimates at various τ were sought for the following set of sixteen λ values:

$$\{0.1, 0.2, 0.4, 1, 2, 4, 10, 20, 40, 100, 200, 400, 1000, 2000, 4000, 10000\}. \quad (9.4)$$

The error shown is the maximum (relative when the ‘exact’ $\rho > 1$, absolute otherwise) over the set of sixteen λ values. For many of these runs the heuristics were overly conservative, but the times are nevertheless quite small. For the Bessel equation of order $\frac{1}{3}$, Example 3 (equation (6.9) with $\nu = 1/3$), the relatively large computing times were due to difficulties near $\lambda = 0$.

Table 9.2. **AutoB results for several tolerances and Four Potentials on $(0, \infty)$.**

Potential	$\tau = 10^{-4}$		$\tau = 10^{-6}$		$\tau = 10^{-8}$		$\tau = 10^{-10}$	
	error	time	error	time	error	time	error	time
1. Ex4($\nu=1$)	1.30(−7)	0.28	1.50(−9)	0.50	1.92(−12)	1.06	1.73(−13)	2.46
2. Ex1($\ell=1$)	1.78(−6)	0.42	7.88(−7)	0.84	1.50(−8)	3.11	7.93(−11)	18.50
3. Ex2($\ell=1$)	2.49(−6)	0.37	3.37(−7)	0.74	8.54(−9)	3.95	1.10(−10)	20.97
4. Ex3($\nu=1/3$)	9.57(−5)	0.49	1.04(−6)	3.00	1.52(−8)	41.95	1.13(−10)	894.77

For comparison, output from the SLEDGE program is shown for the Bessel equation of order Example 4 with $\nu = 1$, Example 4 (equation (6.13) in Table 9.3. Since SLEDGE is known [15] to have difficulty with large values of λ , we ran the program at various choices of τ only on the first n λ -values from (9.4) with $n = 1, 2, \dots, 9$. The final line ($n = 16$) is output from AutoB using all sixteen λ values up to $\lambda = 10000$. Clearly, AutoB is much more reliable than SLEDGE. Similar results were observed for other doubly singular potentials.

Table 9.3. **SLEDGE output for the Bessel equation of order 1**($q(x) = 0.75/x^2$)

n	$\tau = 10^{-3}$		$\tau = 10^{-4}$		$\tau = 10^{-5}$		$\tau = 10^{-6}$	
	error	time	error	time	error	time	error	time
1	1.31(−4)	0.02	3.87(−5)	0.09	9.74(−6)	0.50	9.92(−6)	1.58
2	6.86(−4)	0.02	1.24(−5)	0.23	1.07(−5)	1.31	9.87(−6)	8.43
3	2.72(−4)	0.14	1.32(−5)	0.34	2.95(−5)	2.34	6.70(−6)	>96.53
4	2.71(−4)	0.16	1.79(−4)	0.50	3.20(−5)	8.45	6.70(−6)	>177.28
5	7.16(−4)	0.19	1.79(−4)	0.70	3.20(−5)	16.40		
6	1.92(−3)	0.21	1.79(−4)	1.71	3.20(−5)	29.51		
7	7.04(−3)	0.96	1.83(−4)	7.67	8.65(−5)	51.64		
8	1.47(−2)	1.83	1.83(−4)	11.39	2.18(−4)	75.87		
9	2.23(−2)	>12.00	3.31(−4)	20.48	2.83(−4)	>465.99		
AutoB								
16	3.69(−6)	0.18	1.30(−7)	0.28	5.74(−9)	0.36	1.50(−9)	0.50

To illustrate the superiority of the new code AutoB over SLEDGE we also ran comparisons on timing and accuracy the Hydrogen Atom potential with $\ell = 1$, Example 1 (equation (6.1)). The output values for $\rho(\lambda)$ obtained for each of the sixteen λ values in (9.4) for four choices of the tolerance levels are displayed in Table 9.4. The $>$ in the time needed for SLEDGE indicates that it stopped (too much time) before the user requested input accuracy was achieved. Since SLEDGE could not achieve 10^{-3} -accuracy over the whole range of λ -values, no SLEDGE runs for tighter tolerances are listed. As the data shows, SLEDGE has much difficulty to compute highly accurate results for large values of λ , while the new codes are capable of quite high accuracy in much less computing time. Similar testing for the Hydrogen Atom potential using the F_x^j approximants was also done in the thesis of Mark Schuster [22].

Table 9.4: **Comparison of SLEDGE with AutoB for Hydrogen problem with $\ell = 1$.**

λ	Exact	SLEDGE	AutoB	AutoB	AutoB	AutoB
0.1	0.005621362	0.0056	0.0056	0.00562	0.0056214	0.005621362
0.2	0.010067470	0.0100	0.0100	0.01007	0.0100675	0.010067470
0.4	0.022334469	0.0222	0.0223	0.02233	0.0223345	0.022334470
1.0	0.087358065	0.0867	0.0874	0.08736	0.0873581	0.087358074
2.0	0.298717032	0.2966	0.2987	0.29872	0.2987170	0.298717047
4.0	1.166166722	1.1577	1.1662	1.16617	1.1661667	1.166166736
10.	8.206942681	8.1493	8.2069	8.20694	8.2069402	8.206942643
20.	38.98117554	38.691	38.981	38.9812	38.981169	38.98117542
40.	194.5884791	192.80	194.59	194.588	194.58845	194.5884785
100.	1719.215348	1706.1	1719.2	1719.21	1719.2140	1719.215343
200.	9188.295022	9068.2	9188.3	9188.29	9188.2922	9188.294986
400.	49923.13741	49137.	49923.	49923.1	49923.126	49923.13720
1000.	475962.2250	462178.	475962.	475961.	475962.23	475962.2484
2000.	2644112.132	2479326.	2644120.	2644111.	2644111.6	2644112.120
4000.	14766762.30	13806576.	14766758.	14766759.	14766759.	14766762.23
10000.	144274264.9	112742503	144274122	144274122	144274123	144274264.3
time (sec)		>177.5	0.31	0.42	0.83	3.75
RelErr		10^{-3}	10^{-3}	10^{-4}	10^{-6}	10^{-8}
AbsErr		10^{-3}	10^{-3}	10^{-4}	10^{-6}	10^{-8}

Remark. High accuracy in the spectral function computation for the Bessel equation on $(0, \infty)$, Examples 3 and 4, was also achieved in [15, Sec 4]; this, however, was done by inserting asymptotic formulas for the eigenvalues and eigenfunction norm reciprocals for the Bessel equation on $(0, b]$ into the SLEDGE code (bypassing the SLEDGE computation of these quantities); but, of course, this was not an automatic procedure applicable to other problems with two singular endpoints.

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